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Computations on Internal Blast From Titanium-Cased Charges in Air

by

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for the
Research Department

JULY 1984

NAVAL WEAPONS CENTER
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FOREWORD

This report documents extension of the continuing research effort on internal blast at the Naval Weapons Center to include addition of titanium as the active metal. Work was performed during the period 1982-1984.

This effort was supported by the Naval Air Systems Command (NAVAIR) and was executed by the Naval Weapons Center under the Surface/Aerospace Weaponry Technology Block Program under AIRTASK A32-320J/008B/3F32-300-000 (Appropriation 1721319.41AJ). This airtask provides for continued exploratory development in the air-to-air and air-to-surface mission areas. Mr. H. B. Benefiel, AIR-320E, is the cognizant NAVAIR technology administrator.

This report has been reviewed for technical accuracy by K. J. Graham.

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(U) This report documents the results of adiabatic internal explosions in systems containing a variety of C-H-N-O fuels in air with the addition of titanium as the active metal. For all of the systems studied, the following were found: adiabatic temperature, overpressure, and yield of each product in terms of moles and as partial pressures for the gaseous products.

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INTRODUCTION

Calculations have been reported from the Naval Postgraduate School for the results of adiabatic internal explosions in systems containing a variety of C-H-N-O fuels in air with or without the addition of the active metals magnesium or aluminum.¹⁻⁷ The present study reflects the extension of the studies to titanium as the active metal.

As before, metal and fuel are considered introduced into a constant volume of 1 m³, initially at 25°C. Products are assumed distributed evenly throughout the volume. The process is treated as adiabatic, and the ideal-gas approximation is assumed to hold.

The fuels considered are listed in Table 1, along with a few pertinent properties. Oxygen balance is computed, on a mass-percent basis, as the excess (deficiency, when negative) of oxygen in the fuel relative to the production of water, carbon monoxide, and elemental nitrogen.

In all the following, the symbol C will represent the charge, or mass of fuel, per cubic meter of air and M, the mass of metal (titanium) per cubic meter. Charge-to-metal (C/M) ratios and total concentrations (C + M, in kilograms per cubic meter) were varied over the range 0.1 to 10 for each.

In several of the tables, a code is used to indicate the condensed phases present: L = liquid oxide solution; C = TiC; N = TiN; G = graphite; A = Ti₃O₅; B = TiO₂.

¹ Naval Weapons Center. *Peak Overpressures for Internal Blast*, by G. F. Kinney, R. G. S. Sewell, and K. J. Graham. China Lake, Calif., NWC, June 1979. (NWC TP 6087, publication UNCLASSIFIED.)

² Naval Weapons Center. *Reactive Metals in Internal Explosions: The Combustion of Magnesium in Air*, by R. A. Reinhardt. China Lake, Calif., NWC, February 1978. (NWC TM 3429, publication UNCLASSIFIED.)

³ Naval Weapons Center. *Adiabatic Computation of Internal Blast for Magnesium-Cased Charges in Air*, by R. A. Reinhardt. China Lake, Calif., NWC, April 1979. (NWC TM 3820, GIDEP E202-1481, publication UNCLASSIFIED.)

⁴ Naval Weapons Center. *Adiabatic Computation of Internal Blast for Aluminum-Cased Charges in Air*, by R. A. Reinhardt and A. K. McDonald. China Lake, Calif., NWC, January 1982. (NWC TP 6287, publication UNCLASSIFIED.)

⁵ Naval Weapons Center. *A Working Model for the System Alumina-Magnesia*, by R. A. Reinhardt. China Lake, Calif., NWC, May 1983. (NWC TP 6433, GIDEP E392-0754, publication UNCLASSIFIED.)

⁶ Naval Weapons Center. *Computer Program for Internal Aluminum-Fuel-Air Explosions*, by R. A. Reinhardt. China Lake, Calif., NWC, May 1983. (NWC TP 6449, GIDEP E413-0319, publication UNCLASSIFIED.)

⁷ Naval Postgraduate School. *Internal Explosions of Reactive Aluminum with a PBX in Air*, by R. A. Reinhardt. Monterey, Calif., NPS, August 1983. (NPS-61-83-011-PR, publication UNCLASSIFIED.)

TABLE 1. Properties of the Fuels.

Designation	Name and chemical formula	ΔU_f , 298, kJ/mole	Oxygen balance, to CO + H ₂ O, %
PETN	Pentaerythritol tetranitrate, C ₅ H ₈ N ₄ O ₁₂	-489.8	+ 15
NC	Nitrocellulose, 13.3% N; C ₆ H ₇ N _{2.5} O ₁₀	-812.9	+ 3
HMX	sym-Cyclotetramethylene- tetranitramine, C ₄ H ₈ N ₈ O ₈	+ 77.4	0
Pentolite	50% PETN, 50% TNT; C _{6.16} H _{6.25} N _{3.41} O _{8.5}	-97.9	-5
Comp B	65% RDX, 35% TNT; C _{1.96} H _{2.53} N _{2.22} O _{2.68}	+ 11.47	-9
TNT	2,4,6-Trinitrotoluene, C ₇ H ₅ N ₃ O ₆	+ 30.7	-25
N ₂ H ₄	Hydrazine	-165.0	-100
C ₂ H ₄ O	Ethylene oxide	-47.29	-109
Carbon	Graphite	0	-133
C ₆ H ₁₄	Hexane	+ 100.31	-242

Internal energies of formation are per mole of formula indicated.
Data were taken or computed from Ref. 1.

BASIS OF CALCULATIONS

As is pointed out in Ref. 4, the adiabatic restriction requires that a temperature be found such that the sums of the internal energies of the equilibrium mixture of products at that temperature must equal the initial internal energy of formation of the chosen fuel. The pressure is then computed from the ideal gas law, taking into account the total number of moles of gas present at equilibrium at the temperature. The overpressure is found by subtracting 1 bar.

As before,⁴ thermochemical data are represented by the five-parameter expression

$$U = B_1 + B_2T + B_3T^2 + B_4\ln T + B_5/T$$

where T is the Kelvin temperature. In Table 2 are listed the internal energy parameters for the 25 gaseous and 15 condensed-phase species considered. Those for titanium species were

TABLE 2. Internal Energies of Combustion Products.
 Expressed as a function of $\tau = T/1000$ (in kilokelvins);
 values given in joules/mole: $U(T) = B_1 + B_2\tau + B_3\tau^2 + B_4\ln\tau + B_5/\tau$

Substance	B ₁	B ₂	B ₃	B ₄	B ₅
Ti	310931	11660	75	1364	664
TiO	264015	30151	272	-2961	1040
TiO ₂	-55866	60797	-355	-22628	-4116
Ti +	1029558	29682	-252	-49343	-43618
Ar	-3718	12473	0	0	0
CO	-84115	31136	-25	-6218	24
CO ₂	-361013	56789	67	-9201	1764
H	213029	12473	0	0	0
OH	166505	34786	-88	-20093	-7842
H ₂	136535	32890	313	-21058	-9413
H ₂ O	50545	63224	-395	-45949	-16417
NO	105501	30619	10	-4353	631
N ₂	38785	31651	-61	-7831	-657
O	214445	9604	298	4428	2050
O ₂	32105	29476	662	-6265	-2102
TiC (l)	-617142	62760	0	0	0
TiC (s)	-762144	27917	6225	14807	3981
Ti (l)	-465953	35564	0	0	0
Ti (s)	-695970	-10976	8134	35009	11727
C (s)	-40329	22904	320	10	0
CN ⁻	102390	31551	-69	29	0
CN	691554	38828	740	-37192	-24658
C ₂ H	758476	66613	239	-43882	-20692
C ₂ N	538335	54371	-15	-1052	2404
HCN	284944	62760	-302	-26216	-5947
HNCO	36816	83592	-474	-28281	-4750
HCO	90276	56166	-353	-19233	-2345
CH ₂ O	54534	85563	-609	-32362	-1612
C ₂ H ₂	474890	92019	-27	-42593	-10539
C ₃	906056	48907	282	-16185	-3220
TiO (l)	-1040198	66944	0	0	0
TiO (s)	-1011246	56480	4163	0	0
Ti ₂ O ₃ (l)	-1942190	156900	0	0	0
Ti ₂ O ₃ (s)	-2041671	145104	2725	-30	4248
Ti ₃ O ₅ (l)	-2875209	234304	0	0	0
Ti ₃ O ₅ (s)	-2963674	174570	16844	266	123
TiO ₂ (l)	-1395260	87864	0	0	0
TiO ₂ (s)	-1436271	62766	5687	159	1079
TiN (l)	-770564	62760	0	0	0
TiN (s)	-847427	38404	5099	4361	812

Substances are gaseous unless otherwise specified.

calculated from data in the JANAF tables,⁸ recomputing the data so as to accommodate the universal choice of titanium vapor as the reference state. Parameters for the other species are taken from Ref. 4.

EQUILIBRIUM CONSIDERATIONS

THE SYSTEM TITANIUM-OXYGEN

Unlike magnesium and aluminum, the metals studied earlier, titanium forms a number of solid oxides. The compounds TiO , Ti_2O_3 and TiO_2 are well known, and their formation accords with the solution chemistry of this transition metal. The phase diagram of the system Ti-O is reasonably well established up to the melting point.^{9,10} Maxima in melting point appear to correspond to Ti_2O , Ti_2O_3 , Ti_3O_5 and TiO_2 . TiO appears to melt incongruently. There is extensive solid-solution formation and considerable temperature-dependent polymorphic transition. Oxygen is soluble in titanium metal to the extent of about 25 atom-percent, yielding solid solutions which show metallic conductance. In general, the lower oxides are all nonstoichiometric and show semiconductor properties.

The phase diagram gives no direct evidence regarding the liquid phase, but the appearance is not inconsistent with that of a system with no discontinuities in the liquid phase.

For these reasons, it has been assumed in the present study that the liquid phase in the system Ti-O is continuous; that is, that there is complete miscibility from the metal to the composition TiO_2 . This liquid is assumed to be an ideal solution of the liquids Ti, TiO , Ti_2O_3 , Ti_3O_5 and TiO_2 . Ti_2O was not included since no thermochemical or equilibrium data appear to be available for it.

The complexities of the solid phases have been ignored in the present study. Only a small number of points were at temperatures below the melting-point curve; most of these were for oxygen-rich systems in which solid TiO_2 formed or for carbon-rich systems in which TiC but no oxide at all resulted. Pure solid phases were assumed in those few cases where solid Ti_3O_5 , alone or with TiO_2 , appeared.

In the computer program the presence of "liquid oxide" (that is, the liquid solution of oxygen in titanium) required in part that the temperature be above 2143 K (the melting point of TiO_2 and the highest temperature on the melting-point curve). This criterion was adopted for the sake of simplicity, and proved satisfactory in all but a handful of cases where a liquid was obtained, but below 2143 K. These points were recomputed, now waiving the temperature requirement for liquid oxide. It was found that this change made very little difference (at most a few tenths of a bar) in the computed pressure.

⁸ National Bureau of Standards. *JANAF Thermochemical Tables*, 2nd edition, by D. R. Stull and H. Prophet. Washington, D.C., NBS, June 1971.

⁹ R. C. DeVries and R. Roy, *Am. Ceramic Soc. Bull.*, Vol. 33 (1954), pp. 370-72.

¹⁰ P. G. Wahlbeck and P. W. Gilles, *J. Am. Ceramic Soc.*, Vol. 49 (1966), pp. 180-83.

A set of calculations was carried out for the system TNT-Ti-air using the quite different (and less reasonable) assumption that the liquid oxide phases were completely immiscible with one another and with the liquid metal. Results were appreciably different, as to both adiabatic temperatures and pressures found. The pressures tended to be higher (by up to 12%) even though the temperatures were lower. This result was in accord with the reduction in fugacities accompanying solution formation.

It should be remarked that it was assumed that TiC, TiN and graphite, when present, existed as pure phases.

EQUILIBRIUM DATA

As in the previous study,⁴ equilibrium constants of formation were fitted to the four-parameter equation:

$$\log_{10} K = A_1 + A_2/(A_3 + T) + A_4 T$$

In Table 3 are listed the equilibrium constant parameters for all the species considered (except for the elements in the reference states, for which all the parameters are zero). Those for the titanium species were computed from the JANAF tables,⁸ with the data below 3591 K (the normal boiling point for titanium) recomputed to take into account the choice of titanium vapor as the reference state. (This choice was made to avoid the discontinuities that would otherwise occur at the melting and boiling temperatures of titanium.) Parameters for the other species are taken from Ref. 4.

In application, each K_p (expressed in partial pressures) is first converted to a K_n (in terms of mole numbers). Then for any species the number of moles is given as a known function of K_n and the "master variables": $X = \sqrt{O_2}$; $Y = \sqrt{H_2}$; $Z = \sqrt{N_2}$; Ti; and Acc, which is the activity of carbon (standard state, graphite). (Formulas in the last sentence refer to number of moles.)

EQUILIBRIUM CALCULATIONS

For argon, the mole number is always 0.4036, the number of moles in 1 m³ of air at 298 K, 1 bar. For each of the five remaining elements, a material balance equation may be written representing conservation of the number of moles of atoms of each element. The mole number of each of the chemical species present is a function of those of the elements in standard states and the activity of carbon; hence, five simultaneous equations in five unknowns (the five "master variables" referred to earlier) are obtained.

In actuality the maximum number of unknowns to be considered is four, since $Y = \sqrt{H_2}$ can always be found in closed form as a function of the others. Considering also the phase rule restriction, the number of variables to be solved for is four less the number of condensed phases. The Newton-Raphson method, as described in Ref. 4, is then used to solve this set of simultaneous nonlinear equations.

TABLE 3. Equilibrium Constants of Formation of Products.
 (Base 10 logarithm of the formation constant of the
 indicated substance, expressed as a function of $\tau = T/1000$
 (in kilokelvins): $\log_{10} K = A_1 + A_2/(A_3 + \tau) + A_4\tau$)

Substance	A ₁	A ₂	A ₃	A ₄
TiO	-2.256	23.248	-0.018	-0.133
TiO ₂	-7.510	37.603	-0.008	-0.067
Ti +	4.082	-39.359	0.079	0.027
CO	4.593	6.108	0.030	-0.067
CO ₂	0.087	20.642	0.001	-0.024
H	3.132	-12.016	0.019	0.015
OH	0.769	-1.969	-0.016	-0.015
H ₂ O	-3.056	13.305	0.014	-0.005
NO	0.710	-4.300	0.008	-0.009
O	3.497	-13.439	0.010	0.006
TiC (l)	-6.352	29.181	-0.002	0.019
TiC (s)	-8.124	33.929	-0.003	0.118
Ti (l)	-6.033	21.383	-0.060	-0.006
Ti (s)	-7.550	24.361	0.000	0.165
CN ⁻	0.826	0.005	-2.418	0.047
CN	5.092	-22.218	-0.012	-0.016
C ₂ H	4.529	-24.269	-0.012	-0.043
C ₂ N	7.060	-29.343	-0.000	-0.066
HCN	1.607	-6.807	-0.012	-0.008
HNCO	-25.740	96.491	2.563	2.862
HCO	2.221	1.209	0.219	-0.060
CH ₂ O	-2.036	6.770	0.018	-0.016
C ₂ H ₂	2.655	-11.332	-0.016	0.000
C ₃	10.850	-41.395	-0.016	-0.186
TiO (l)	-8.512	44.816	-0.050	0.052
TiO (s)	11.560	50.682	-0.009	0.348
Ti ₂ O ₃ (l)	-22.269	112.701	-0.054	0.030
Ti ₂ O ₃ (s)	-28.610	126.047	-0.007	0.607
Ti ₃ O ₅ (l)	-36.762	182.554	-0.039	0.085
Ti ₃ O ₅ (s)	-45.523	200.007	-0.003	0.984
TiO ₂ (l)	-13.912	66.399	-0.042	0.042
TiO ₂ (s)	-17.167	73.460	-0.003	0.290
TiN (l)	-5.271	20.076	-0.672	-0.437
TiN (s)	-12.371	41.581	-0.007	0.196

Substances are gaseous unless otherwise specified.

An initial approximation scheme is available wherein it is assumed that oxygen is taken up in the order CO , TiO_x , H_2O , CO_2 . With insufficient oxygen to proceed beyond TiO , TiN is assumed. With excess carbon, TiC or C (solid) is assumed. Based on these assumptions, initial values of all the master variables can be found and the computation may be started. After the first computation in a series it is a matter of operator choice whether to repeat the initial approximation or to use the values of the master variables from the last run.

In any case, after convergence of the Newton's method of calculation, tests are performed for the presence or absence of each condensed phase. If a change from those assumed has occurred the computation is rerun. This procedure continues until all the tests are satisfied and no change in condensed phases is predicted. Further detail on the computational method with a copy of the computer program is given in Appendixes A and B to this report.

RESULTS

For all the systems studied the following were found: adiabatic temperature, overpressure, and yield of each product in terms of moles and also as partial pressures for the gaseous products. Total concentration (metal plus fuel) was varied regularly over the range 0.1 to 10 kg/m^3 and the fuel-to-metal ratio likewise was varied over the range 0.1 to 10.

In Table 4 the following data are given for titanium plus air (in the absence of fuel): overpressures (bars), adiabatic temperatures (K), and product yields, expressed as mole-percent for the gases and total mole number for condensed phases. The composition of the liquid oxide phase is given as x in the empirical formula TiO_x (x ranging from 0 to 2).

TABLE 4. Combustion of Pure Titanium in Air:
Overpressure, Adiabatic Temperature, and Product Yield.

Property/ system	Concentration, kg/m^3						
	0.1	0.2	0.4	1.0	2.0	4.0	10.0
Overpressure, bars	7.3	9.7	11.7	14.3	18.4	26.3	49.8
Temperature, K	2602	3423	4024	4338	4393	4542	4869
Mole-%:							
Ar	1.05	1.08	1.07	0.95	0.76	0.56	0.32
Ti	0.01	7.22	30.08	50.59	72.46
TiO	...	0.12	4.86	17.42	9.85	5.22	2.15
TiO ₂	...	0.01	0.08
NO	2.47	5.05	4.09	0.05	0.01
N ₂	80.84	81.46	81.12	74.26	59.59	43.63	25.06
O	0.32	3.64	6.54	0.10	0.01	0.01	...
O ₂	15.31	8.64	2.23
Liquid oxide:							
Moles	2.04	2.77	4.55	10.40	20.55	43.2	115.0
x in TiO_x	1.99	1.79	1.40	0.91	0.57	0.31	0.12

Table 5 gives overpressures in bars, with the temperature in parentheses, for the titanium-air-fuel mixtures. Each portion of the table is devoted to a particular fuel, and the fuels are arranged in decreasing order of oxygen balance, starting with the most oxygen-rich, PETN, and ending with the most oxygen-deficient, hexane. In each case, $C + M$ represents the total concentration in kilogram/meter³, and C/M represents the mass ratio of fuel to metal. For each table entry a code indicates the condensed phases present; this code, described earlier, is also explained as a footnote to the table.

TABLE 5. Overpressure (in bars), Adiabatic Temperature (in K) (in parentheses), and Condensed Phases for the Combustion of Titanium With Fuels in Air.

$C + M$	C/M						
	0.1	0.2	0.4	1.0	2.0	4.0	10.0
a. Fuel: PETN.							
0.1	7.1 (2496) L	6.8 (2403) L	6.4 (2249) L	5.8 (2004) B	5.1 (1743) B	4.4 (1527) B	3.8 (1344) B
0.2	9.6 (3314) L	9.5 (3228) L	9.3 (3095) L	8.9 (2832) L	8.2 (2564) L	7.5 (2286) L	6.7 (2041) B
0.4	11.9 (3947) L	12.1 (3874) L	12.2 (3739) L	12.1 (3450) L	11.8 (3209) L	11.5 (2995) L	11.0 (2776) L
1.0	15.4 (4363) L	16.3 (4335) L	17.5 (4253) L	19.1 (4033) L	19.6 (3788) L	19.6 (3554) L	19.4 (3349) L
2.0	20.7 (4438) L	22.6 (4486) L	25.6 (4549) L	29.7 (4349) L	31.6 (4107) L	32.3 (3861) L	32.4 (3635) L
4.0	31.3 (4586) L	35.3 (4639) L	41.7 (4743) L	51.4 (4674) L	55.8 (4390) L	57.7 (4116) L	58.3 (3865) L
10.0	63.2 (4913) L	74.4 (4970) L	91.9 (5098) L	121.0 (5177) L	132.1 (4773) L	136.4 (4426) L	138.0 (4127) L

L = liquid oxide, B = TiO_2 (s).

TABLE 5. (Contd.).

C + M	C/M						
	0.1	0.2	0.4	1.0	2.0	4.0	10.0
b. Fuel: Nitrocellulose.							
0.1	7.1 (2508) L	6.9 (2427) L	6.6 (2294) L	6.1 (2089) B	5.4 (1863) B	4.9 (1676) B	4.4 (1520) B
0.2	9.6 (3322) L	9.5 (3244) L	9.4 (3125) L	9.1 (2903) L	8.7 (2696) L	8.2 (2488) L	7.6 (2285) L
0.4	11.9 (3949) L	12.1 (3880) L	12.3 (3756) L	12.3 (3497) L	12.2 (3289) L	12.0 (3118) L	11.8 (2965) L
1.0	15.4 (4347) L	16.4 (4324) L	17.7 (4246) L	19.4 (4045) L	20.2 (3829) L	20.4 (3625) L	20.4 (3451) L
2.0	20.8 (4408) L	22.8 (4428) L	25.8 (4467) L	30.3 (4339) L	32.5 (4120) L	33.6 (3902) L	34.0 (3703) L
4.0	31.3 (4550) L	35.4 (4568) L	41.8 (4610) L	52.9 (4649) L	57.8 (4389) L	60.2 (4137) L	61.2 (3908) L
10.0	63.0 (4870) L	73.9 (4884) L	91.2 (4922) L	122.9 (5040) L	137.9 (4775) L	143.0 (4436) L	145.2 (4150) L
c. Fuel: HMX.							
0.1	7.0 (2492) L	6.8 (2396) L	6.4 (2235) L	5.7 (1977) B	4.9 (1706) B	4.3 (1481) B	3.6 (1290) B
0.2	9.6 (3311) L	9.5 (3222) L	9.3 (3084) L	8.8 (2808) L	8.1 (2519) L	7.3 (2218) L	6.5 (1956) B
0.4	11.9 (3944) L	12.1 (3869) L	12.2 (3731) L	12.1 (3431) L	11.8 (3175) L	11.4 (2943) L	10.7 (2697) L
1.0	15.4 (4340) L	16.3 (4313) L	17.6 (4225) L	19.1 (3999) L	19.6 (3744) L	19.5 (3491) L	19.2 (3267) L
2.0	20.8 (4396) L	22.7 (4406) L	25.7 (4429) L	29.9 (4287) L	31.7 (4032) L	32.2 (3765) L	32.0 (3514) L
4.0	31.2 (4536) L	35.2 (4540) L	41.4 (4560) L	52.1 (4579) L	56.2 (4285) L	57.5 (3979) L	57.4 (3691) L
10.0	62.8 (4852) L	73.3 (4849) L	89.9 (4857) L	119.9 (4910) L	133.7 (4639) L	135.7 (4236) L	135.0 (3879) L

L = liquid oxide, B = TiO₂ (s).

TABLE 5. (Contd.).

C + M	C/M						
	0.1	0.2	0.4	1.0	2.0	4.0	10.0
d. Fuel: Pentolite.							
0.1	7.1 (2510) L	6.9 (2431) L	6.6 (2301) L	6.1 (2102) B	5.5 (1881) B	5.0 (1698) B	4.5 (1545) B
0.2	9.6 (3324) L	9.5 (3247) L	9.4 (3130) L	9.1 (2914) L	8.7 (2715) L	8.3 (2517) L	7.7 (2323) L
0.4	11.9 (3951) L	12.1 (3883) L	12.3 (3762) L	12.3 (3505) L	12.2 (3297) L	12.1 (3130) L	11.8 (2983) L
1.0	15.4 (4334) L	16.4 (4313) L	17.6 (4236) L	19.4 (4037) L	20.1 (3822) L	20.3 (3613) L	20.3 (3432) L
2.0	20.7 (4385) L	22.6 (4384) L	25.6 (4389) L	30.3 (4311) L	32.5 (4091) L	33.4 (3863) L	33.6 (3647) L
4.0	31.1 (4523) L	35.0 (4514) L	41.1 (4508) L	52.0 (4517) L	57.8 (4343) L	59.8 (4071) L	60.3 (3811) L
10.0	62.3 (4839) L	72.4 (4822) L	88.3 (4800) L	117.3 (4778) L	137.8 (4710) L	142.1 (4345) L	142.1 (4000) L
e. Fuel: Comp B.							
0.1	7.1 (2503) L	6.9 (2418) L	6.5 (2277) L	6.0 (2056) B	5.3 (1817) B	4.7 (1618) B	4.2 (1452) B
0.2	9.6 (3319) L	9.5 (3238) L	9.4 (3113) L	9.0 (2876) L	8.5 (2648) L	7.9 (2414) L	7.3 (2188) L
0.4	11.9 (3948) L	12.1 (3877) L	12.3 (3750) L	12.3 (3477) L	12.1 (3252) L	11.8 (3065) L	11.5 (2893) L
1.0	15.5 (4326) L	16.4 (4302) L	17.7 (4220) L	19.3 (4009) L	20.0 (3776) L	20.0 (3546) L	19.9 (3344) L
2.0	20.8 (4373) L	22.7 (4362) L	25.6 (4350) L	30.3 (4270) L	32.2 (4029) L	32.8 (3771) L	32.7 (3520) L
4.0	31.1 (4509) L	35.0 (4488) L	40.9 (4460) L	51.4 (4421) L	57.4 (4264) L	58.6 (3949) L	58.2 (3632) L
10.0	62.2 (4822) L	72.2 (4791) L	87.5 (4743) L	114.9 (4655) L	135.4 (4567) L	139.0 (4187) L	135.6 (3756) L

L = liquid oxide, B = TiO₂ (s).

TABLE 5. (Contd.).

C + M	C/M						
	0.1	0.2	0.4	1.0	2.0	4.0	10.0
f. Fuel: TNT.							
0.1	7.1 (2524) L	7.0 (2459) L	6.7 (2352) L	6.2 (2147) L	5.9 (2013) B	5.5 (1862) B	5.1 (1736) B
0.2	9.6 (3334) L	9.5 (3265) L	9.5 (3163) L	9.3 (2982) L	9.1 (2832) L	8.9 (2695) L	8.6 (2565) L
0.4	12.0 (3954) L	12.2 (3891) L	12.4 (3780) L	12.6 (3547) L	12.5 (3355) L	12.4 (3205) L	12.3 (3082) L
1.0	15.5 (4298) L	16.4 (4264) L	17.8 (4195) L	19.6 (3995) L	20.4 (3776) L	20.5 (3537) L	20.2 (3292) L
2.0	20.7 (4331) L	22.5 (4281) L	25.2 (4201) L	29.5 (4037) L	32.3 (3874) L	33.3 (3641) L	31.8 (3252) L
4.0	30.8 (4463) L	34.3 (4404) CL	39.4 (4352) CL	48.1 (4194) CL	53.6 (3979) CL	56.1 (3682) CL	54.8 (3259) CL
10.0	60.7 (4812) CL	69.2 (4791) CL	82.7 (4732) CL	106.0 (4531) CL	120.7 (4244) CL	126.2 (3833) CL	122.3 (3286) CL
g. Fuel: Hydrazine.							
0.1	7.2 (2510) L	7.1 (2437) L	6.9 (2320) L	6.6 (2143) B	6.1 (1961) B	5.8 (1809) B	5.4 (1684) B
0.2	9.7 (3303) L	9.8 (3227) L	9.9 (3118) L	10.0 (2921) L	9.9 (2750) L	9.7 (2589) L	9.4 (2436) L
0.4	12.3 (3899) L	12.7 (3805) L	13.3 (3659) L	14.0 (3386) L	14.2 (3141) L	14.0 (2895) L	13.5 (2644) L
1.0	17.0 (4277) L	18.8 (4146) L	21.2 (3983) L	23.4 (3555) L	22.8 (3005) L	20.8 (2457) L	18.3 (1979) A
2.0	23.4 (4252) L	27.0 (4152) L	32.0 (3991) L	39.0 (3626) L	39.1 (3042) L	29.9 (2047) A	28.2 (1739) AB
4.0	36.2 (4373) L	43.3 (4248) L	53.4 (4104) NL	68.0 (3735) NL	70.9 (3101) NL	55.3 (2062) NL	43.7 (1443) AD
10.0	75.6 (4650) L	93.8 (4482) L	119.9 (4374) NL	157.9 (3927) NL	165.0 (3148) NL	130.3 (2068) NL	93.1 (1291) AN

L = liquid oxide, A = Ti_3O_5 (s), B = TiO_2 (s), C = TiC, N = TiN

TABLE 5. (Contd.).

C + M	C/M						
	0.1	0.2	0.4	1.0	2.0	4.0	10.0
h. Fuel: Ethylene oxide.							
0.1	7.3 (2580) L	7.4 (2568) L	7.5 (2551) L	7.6 (2523) L	7.8 (2502) L	7.9 (2487) L	7.9 (2475) L
0.2	9.8 (3354) L	10.0 (3314) L	10.2 (3261) L	10.6 (3175) L	10.9 (3103) L	11.1 (3034) L	11.2 (2963) L
0.4	12.3 (3929) L	12.8 (3857) L	13.4 (3743) L	14.3 (3502) L	14.5 (3246) L	14.2 (2975) L	13.7 (2711) L
1.0	16.6 (4194) L	18.2 (4083) L	20.3 (3903) L	22.7 (3551) CL	23.5 (3220) CLN	22.4 (2760) CN	18.9 (2164) CG
2.0	22.6 (4207) L	25.4 (4085) CL	29.3 (3984) CL	35.0 (3676) CL	37.3 (3252) CL	32.9 (2578) CG	29.6 (2133) CG
4.0	34.1 (4374) CL	39.6 (4318) CL	47.9 (4204) CL	59.9 (3820) CL	62.6 (3268) C	57.0 (2612) CG	51.1 (2115) CG
10.0	68.9 (4741) CL	83.3 (4676) CL	105.1 (4535) CL	136.2 (4022) CL	136.8 (3259) C	129.8 (2648) CG	115.8 (2107) CG
i. Fuel: Carbon.							
0.1	7.4 (2616) L	7.5 (2627) L	7.6 (2643) L	7.8 (2667) L	7.9 (2678) L	8.0 (2678) L	8.1 (2671) L
0.2	9.8 (3404) L	9.9 (3386) L	10.0 (3350) L	10.2 (3241) L	9.9 (3038) L	9.0 (2657) L	7.8 (2260) L
0.4	12.1 (3979) L	12.3 (3929) L	12.6 (3792) L	12.1 (3336) N	10.5 (2821) CG	8.4 (2305) CG	7.0 (1960) GN
1.0	15.2 (4067) L	15.3 (3908) CL	15.2 (3804) CL	13.8 (3588) CG	11.2 (3010) CG	8.0 (2221) CG	5.8 (1709) GN
2.0	19.2 (4168) CL	19.1 (4126) CL	20.0 (4473) C	15.0 (3788) CG	11.7 (3128) CG	7.8 (2170) CG	5.1 (1558) GN
4.0	26.5 (4414) CL	26.1 (4375) CL	24.5 (4716) C	16.4 (3962) CG	12.1 (3212) CG	7.7 (2135) CG	3.5 (1421) AGN
10.0	48.2 (4792) CL	47.8 (5133) C	36.4 (5014) C	18.9 (4165) CG	12.3 (3276) CG	7.6 (2110) CG	2.4 (1365) AGN

L = liquid oxide, C = TiC, G = graphite, N = TiN, A = Ti₃O₅ (s)

TABLE 5. (Contd.).

C + M	C/M						
	0.1	0.2	0.4	1.0	2.0	4.0	10.0
j. Fuel: Hexane.							
0.1	7.6 (2650) L	7.8 (2691) L	8.2 (2749) L	8.9 (2824) L	9.3 (2850) L	9.6 (2833) L	9.6 (2771) L
0.2	10.1 (3387) L	10.4 (3373) L	10.9 (3336) L	11.4 (3127) L	11.0 (2757) L	10.1 (2391) L	9.3 (2082) L
0.4	12.7 (3902) L	13.4 (3794) L	14.4 (3572) L	14.7 (3037) LN	12.7 (2359) CN	10.8 (1925) GN	9.1 (1552) GN
1.0	17.4 (4005) L	18.9 (3805) CLN	20.8 (3629) CLN	20.2 (2826) C	17.7 (2184) CG	15.3 (1760) GN	12.6 (1377) ABG
2.0	23.6 (4075) CL	26.6 (3972) CL	30.7 (3740) CL	30.5 (2891) CG	27.3 (2162) CG	23.3 (1674) GN	19.2 (1297) BG
4.0	35.8 (4293) CL	42.3 (4177) CL	52.2 (4042) C	51.3 (2951) CG	46.5 (2151) CG	39.4 (1622) GN	31.9 (1205) BG
10.0	73.4 (4623) CL	90.2 (4481) CL	111.5 (4276) C	113.7 (3009) CG	104.3 (2146) CG	88.2 (1586) GN	64.2 (1025) BGN

L = liquid oxide, A = Ti_3O_5 (s), B = Ti_3O_5 (s), C = TiC , G = graphite, N = TiN

In Table 6 is given the set of product yields for TNT-titanium-air at $C/M = 1.0$, chosen as representative. Mole-percent in the vapor is given for each species that reaches at least 0.1% at some point. Numbers of moles of condensed phases are also given. As with Table 4, the composition of the liquid oxide phase is given as x in the empirical formula TiO_x .

Product-yield data are available for all the systems run but have not been included in this report due to the bulk of data involved. They are available from the author.

DISCUSSION

Figure 1 shows the effect of total concentration ($C + M$) on adiabatic temperature for pure titanium in air as well as for two representative C/M ratios for the oxygen-deficient hexane and the oxygen-rich nitrocellulose.

**TABLE 6. Combustion of TNT-Titanium in Air at $C/M = 1.0$:
Overpressure, Adiabatic Temperature, and Product Yields.**

Property/ system	$C + M, \text{ kg/m}^3$						
	0.1	0.2	0.4	1.0	2.0	4.0	10.0
Overpressure, bars	5.2	9.3	12.5	19.6	29.5	48.1	106.0
Temperature, K	2147	2982	3547	3995	4037	4194	4531
Mole %:							
Ar	0.99	0.97	0.88	0.65	0.44	0.29	0.14
Ti	0.03	4.47	6.80	7.84
TiO	0.31	4.35	3.22	2.41	2.57
TiO ₂	0.02	0.02
Ti+	0.01	0.01
CO	0.01	1.82	9.79	24.20	33.46	37.91	40.95
CO ₂	3.78	5.58	3.62	0.62
H	...	0.14	1.53	7.02	8.55	10.01	12.30
OH	0.08	1.02	2.19	0.91	0.01	...	0.01
H ₂	...	0.09	0.74	4.03	7.65	10.06	12.22
H ₂ O	1.31	1.97	2.19	0.87	0.01	0.01	0.01
NO	0.99	3.08	3.14	0.62
N ₂	77.86	75.58	69.80	55.73	41.72	31.12	21.69
O	0.03	0.98	2.66	0.89
O ₂	14.94	8.78	3.13	0.08
CN ⁻	0.01	0.01
CN	0.09	0.25	0.46
C ₂ H	0.01	0.06	0.20
C ₂ N	0.02	0.06
HCN	0.34	0.97	1.52
HNCO	0.01
HCO	0.01	0.01	0.03	0.06
C ₂ H ₂	0.03	0.11
Liquid oxide:							
Moles	1.04	1.70	2.58	6.48	13.88	22.60	45.39
x in TiO _x	2.00	1.94	1.69	1.18	0.72	0.57	0.56
Moles TiC (l)	6.17	29.86

The behavior of the pure metal is quite unlike that previously seen for aluminum (where a maximum in T versus $C + M$ occurred at approximately the Al_2O_3 stoichiometry; see Ref. 4). With titanium there is a steady increase in temperature with concentration, the result of the existence of a number of oxides, the formation of each being an exothermic process. Again, whereas aluminum showed formation of AlN at high concentrations, TiN does not form here as a product owing to the lesser high-temperature stability of TiN . The

curves for the explosive (relatively oxygen-rich) fuels are very similar to those for the metal alone.

With the oxygen-deficient fuels, first TiN and then TiC and graphite appear as products in the carbon-rich region. These tend to cause a falling off of temperature, as is seen in the case of hexane in Figure 1.

Figure 2 shows the strong effect of total concentration on overpressure. Nitrocellulose has been chosen as representative; all the fuels (except carbon) show a similar pattern. The large increase in number of moles of gaseous products combined with a much less profound change in temperature (Figure 1) is responsible for the monotonic increase in pressure.

The effect of C/M on temperature is shown in Figure 3. In general, titanium has a higher heating value than any of the fuels used; hence, there is a generally observed decrease in temperature as titanium is replaced by fuel. At high concentrations with oxygen-rich fuels, the oxygen supplied by the fuel causes the temperature to rise at first, resulting in a shallow maximum in the curve. The considerable break downward in the curves for hexane again corresponds to the production of TiC and graphite.

Commonly, overpressure increases with C/M , as seen in Figure 4, owing to the increase in number of moles of gases ($\text{CO} + \text{H}_2$) as titanium is replaced by fuel. The maximum seen with hexane reflects the sharp drop in temperature, referred to above.

The nature of the fuel has little effect on the adiabatic temperature for the oxygen-rich fuels. For the oxygen-deficient fuels there is a general increase in temperature as the oxygen balance increases (becomes less negative), as is shown in Figure 5, presumably due to relieving the oxygen lack. Pressure is surprisingly insensitive to the nature of the fuel, except for the case of carbon which shows higher temperatures and markedly lower pressures as a result of a much smaller quantity of gaseous product than with the hydrogen-containing fuels. Carbon also shows a very different set of products from those represented in Table 6. With carbon at high concentrations are seen large amounts of CN, C_2N and C_3 and even several tenths mole-percent of the ions as a result of the high temperatures experienced, combined with the absence of hydrogen.

APPROXIMATIONS

Athow has examined¹¹ the ideal-gas approximation for computation on internal explosions in the presence of the reactive metal aluminum. In those systems it appears that the only gas below its critical temperature is aluminum vapor; and for aluminum⁷ the reduced pressure can be seen not to exceed 10^{-4} and the reduced volume not to be less than 200 so that no appreciable deviation from ideality should occur. It is anticipated that the same conclusions can be made regarding the titanium systems, although no estimates of the critical properties have been made and thus no estimates of errors attempted.

¹¹ L. K. Athow, "Real Gas Considerations for Determining Physical and Thermodynamic Properties of Gases Involved in the Prediction of the Effects of Internal Explosions." M. S. Thesis, Naval Postgraduate School, Monterey, Calif., June 1982.

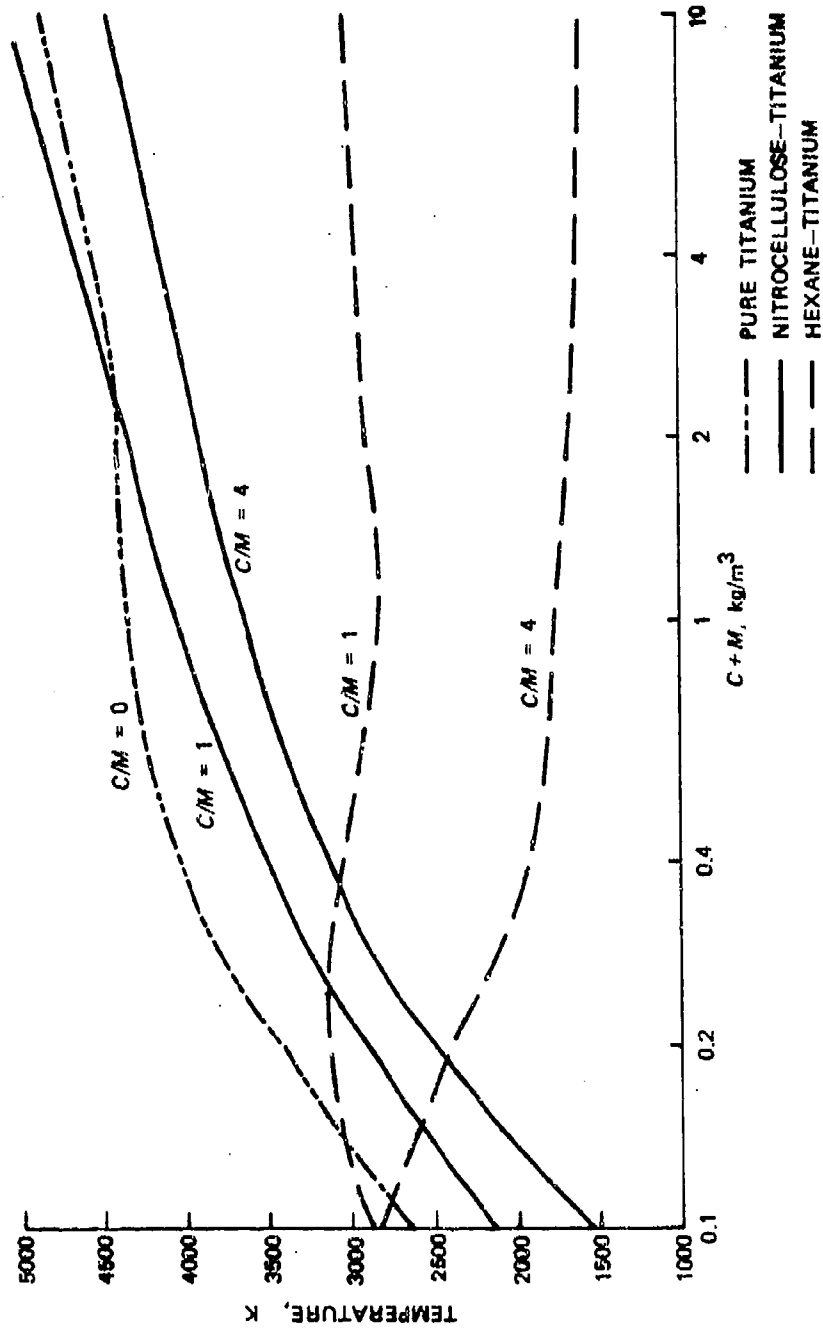


FIGURE 1. Adiabatic Temperature vs. Total Concentration for Pure Titanium; for Nitrocellulose-Titanium; and for Hexane-Titanium in Air.

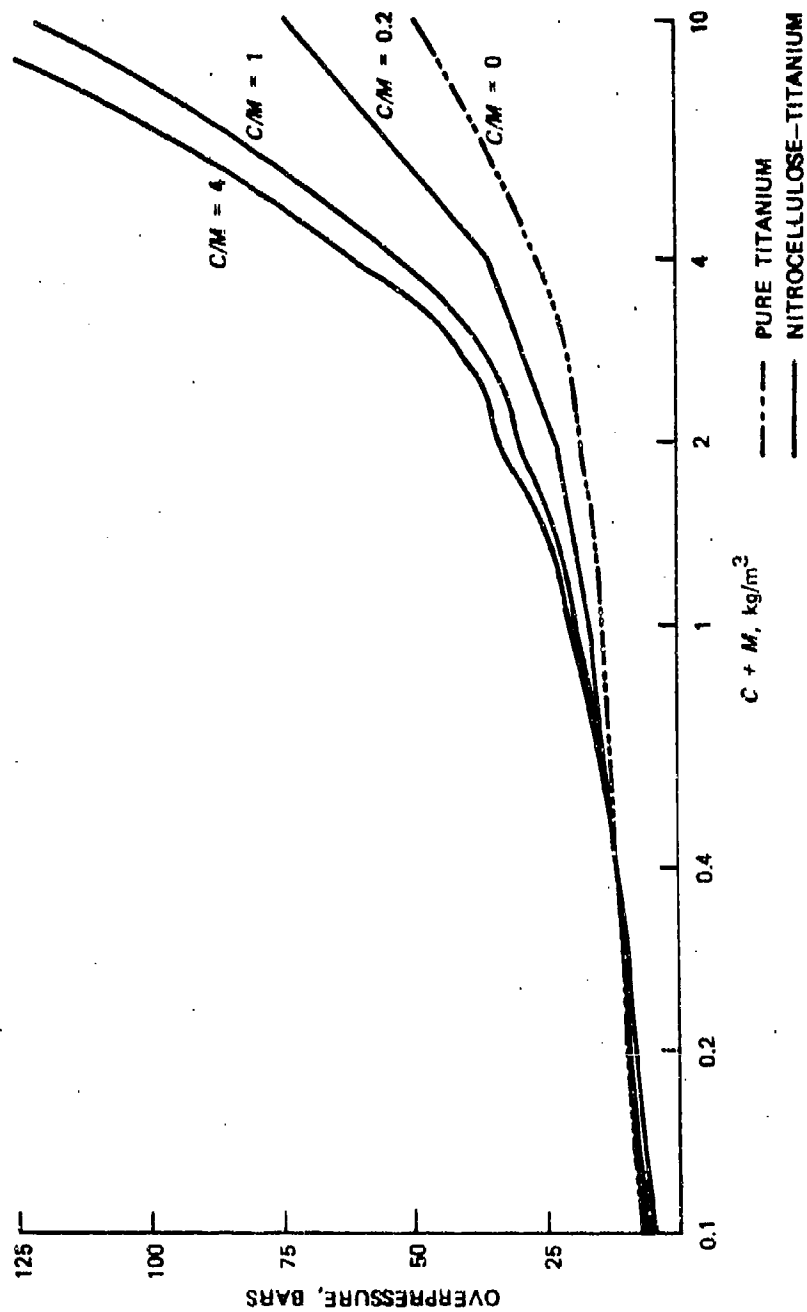


FIGURE 2. Overpressure vs. Total Concentration for Pure Titanium and for Nitrocellulose-Titanium in Air.

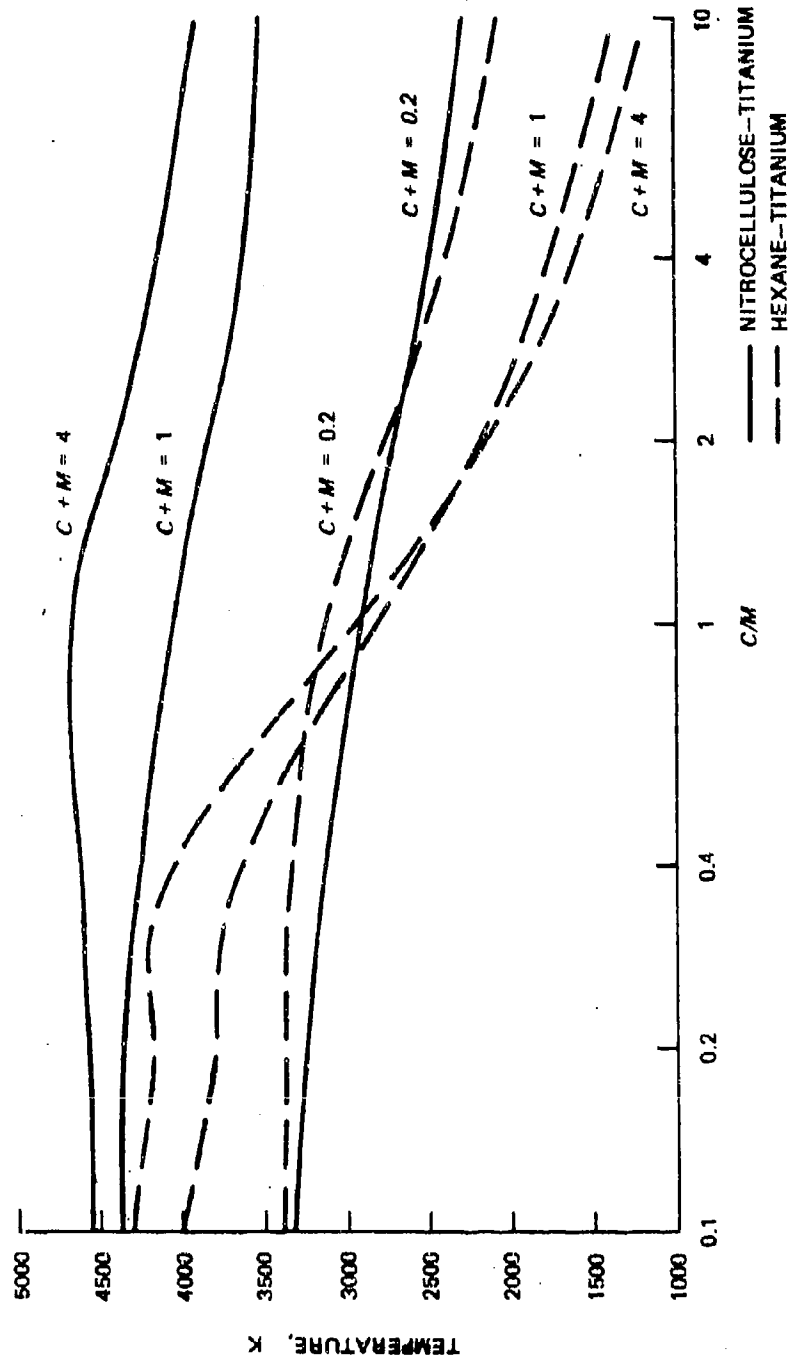


FIGURE 3. Adiabatic Temperature vs. Charge-to-Metal Ratio for Nitrocellulose and Hexane with Titanium in Air.

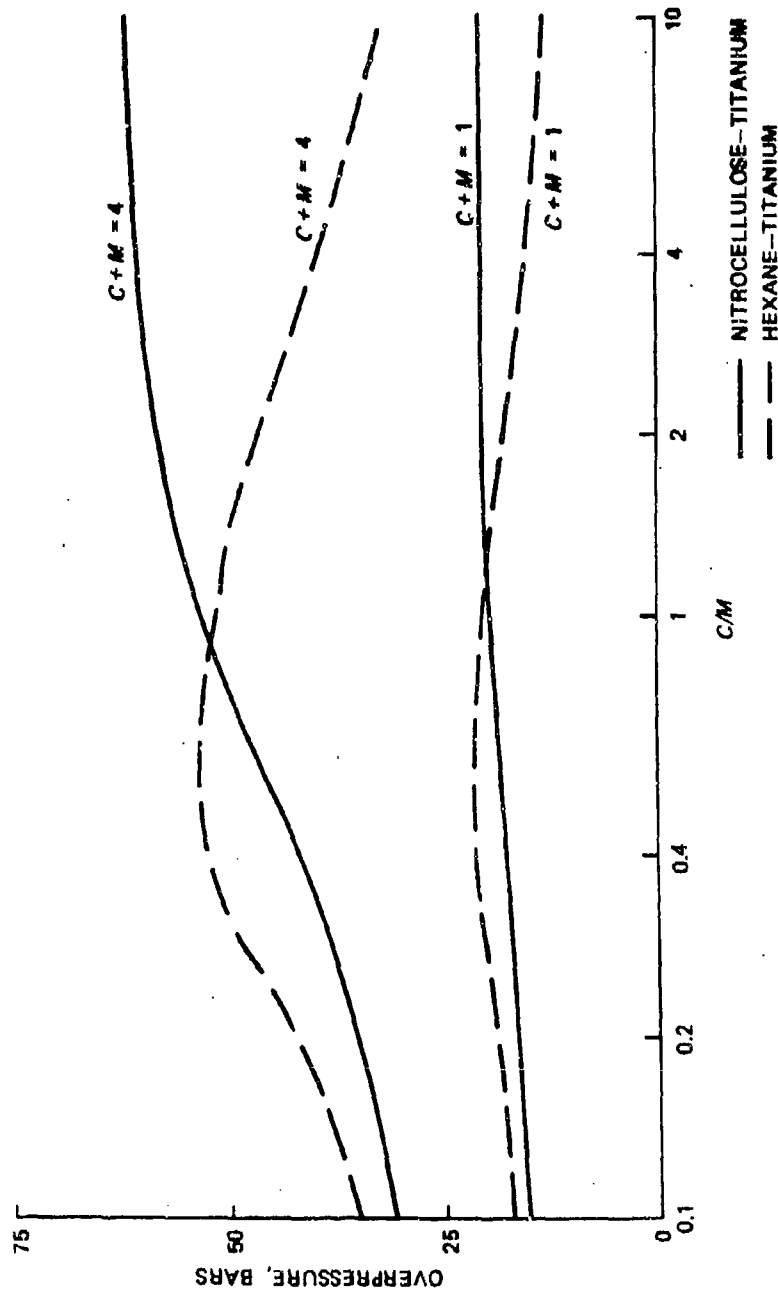


FIGURE 4. Overpressure vs. Charge-to-Metal Ratio for Nitrocellulose and Hexane with Titanium in Air.

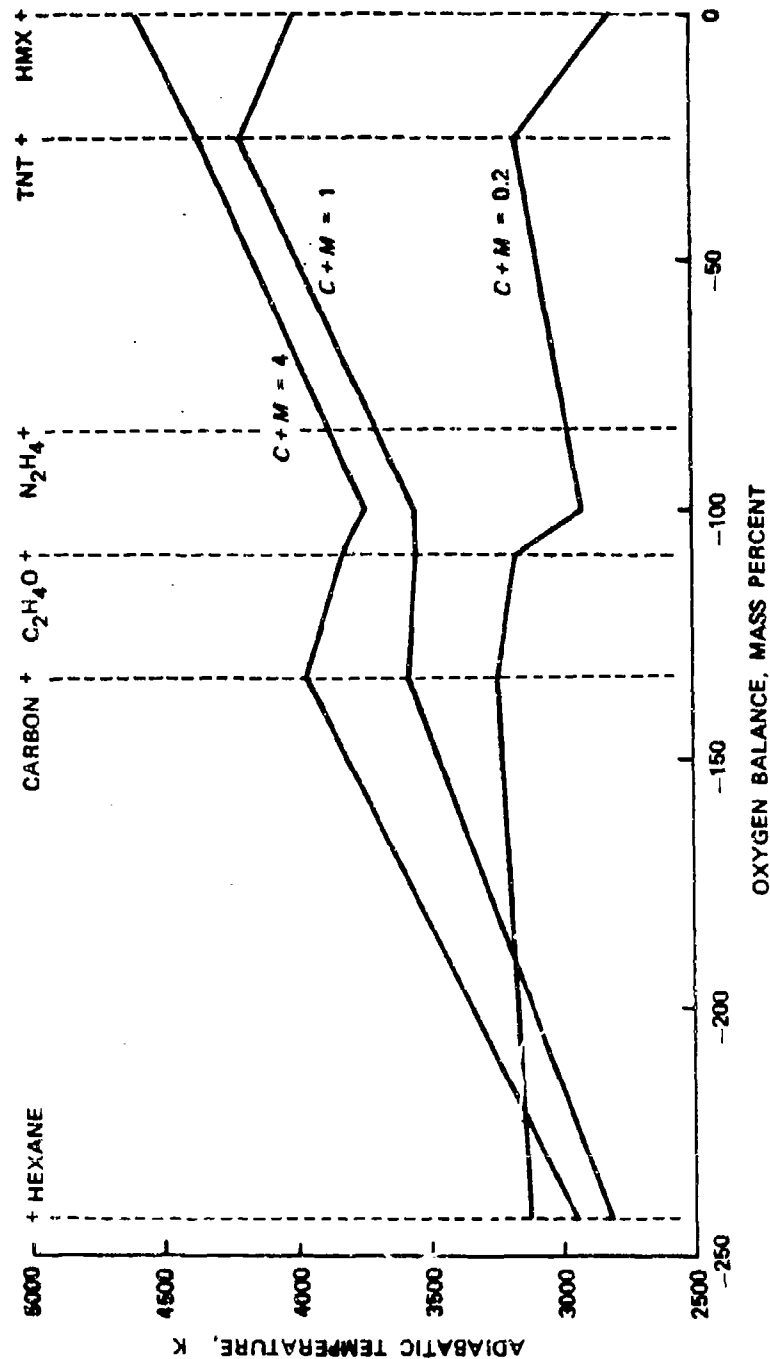


FIGURE 5. Adiabatic Temperature vs. Oxygen Balance for the Combustion of Six Fuels at $C/M = 1.0$ in the Presence of Titanium and Air.

It was pointed out by Smith¹² that radiation effects should be negligible when detonation takes place. When the combustion is a deflagration, however, the adiabatic assumption is expected to be less reliable. A comparison of the experimental data on dust explosions reported by the Bureau of Mines¹³ would seem to show that the computed results from the present report may be high by a factor of about two. It has, however, been pointed out by Baker *et al.*¹⁴ that the Hartmann apparatus used by the Bureau of Mines investigators seriously underestimates the maximum overpressures to be expected. On this basis it is anticipated that the adiabatic results will show much less extreme negative departures from realistic maximum overpressures.

¹² D. E. Smith, "Attenuation Effects of Thermal Radiation on Internal Blast Overpressure." M. S. Thesis, Naval Postgraduate School, Monterey, Calif., December 1979.

¹³ Bureau of Mines. *Explosibility of Metal Powders*, by M. Jacobson, A. R. Cooper and J. Nagy. U.S. Department of Interior, Washington, D.C., 1964. (RI 6516, publication UNCLASSIFIED.)

¹⁴ W. E. Baker, P. A. Cox, P. S. Westine, J. J. Kulesz, and R. A. Strehlow. *Explosion Hazards and Evaluation*. Amsterdam, Elsevier, 1982, pp. 260-61.

Appendix A DESCRIPTION OF THE COMPUTER PROGRAM

The program itself, which is listed in Appendix B, is written for the HP 9845A computer. Various sections are referred to by their labels.

MAIN PROGRAM

Input Section

Fuel (accessible from line 1900). Enter formula and internal energy of formation. Computes formula mass; allows for zero C or H or no fuel. Resets flags.

Conc (accessible from line 1870). Resets counters. Enter $C + M$ (total concentration in kg/m^3) and then C/M , as asked for.

Temp (for entering total temperature manually). May be accessed by use of special function key k4. After at least two trials, **Temp** may be bypassed and interpolation used to find the new temperature. Pressing k5, so that $\text{At\$} = \text{"Y"}$, after two iterations allows for automatic interpolation. If needed, the automatic interpolation may be stopped by pressing PAUSE, then k5 (which returns $\text{At\$}$ to "N"), and finally k4 for manual setting of temperature.

Computation Section

Calc calls up the computational subroutines **Eq**, **Tical**, and **Ex**.

Eq is a subroutine of the main program to evaluate equilibrium constants of formation of each of the 40 chemical species. K_p is first computed from the stored parameters and then converted to K_n (expressed in mole numbers). K_p or K_n is defined as the ratio of the activity of the species to the product of the activities of C, Ti vapor, H_2 , N_2 , and O_2 , each raised to the appropriate power. For Ti_2O_3 and Ti_3O_5 , $\sqrt{K_n}$ is computed so as to avoid overflow at lower temperatures. For condensed phases, the standard state is the pure phase; for K_n , the standard state for gases is 1 mole (in 1 m^3).

Tical is the master subroutine which carries out equilibrium and energy calculations. Results are displayed as "dU" (net) and "T high" or "T low"; $dU = 0$ is desired for convergence. A new temperature approximation is performed automatically by interpolation, based on the previous T and dU values; or else it is entered manually with k4. A more detailed description of **Tical** will be found below.

Output

At Ex, results of the calculations are printed: temperature, overpressure, mole numbers of all products and the diagnostic features described under DIAGNOSTICS, below. Options are allowed at this point for changing C/M, C + M or for a new fuel.

SUBROUTINE TICAL

Tical is the major computational subroutine whose task is to find the numbers of moles of the products present at equilibrium at the selected temperature. The conditions to be satisfied (other than for the trivial case of argon) are the atom balances in C, H, N, O, and Ti and the establishment of chemical equilibrium between each compound and its component elements in their reference states.

The master variables (all in mole numbers) are $X = \sqrt{O_2}$, $Y = \sqrt{H_2}$, $Z = \sqrt{N_2}$, Acc = activity of carbon (standard state = graphite), and Ti = Ti metal vapor. Of these, Y is always computed in closed form; from one to four of the remaining are found as unknown parameters in the subroutine Newt by using the Newton-Raphson method. The actual number of unknowns is equal to four, reduced by the number of condensed phases present. Possible condensed phases are: Ti (solid), TiO (solid), Ti_2O_3 (solid), Ti_3O_5 (solid), TiO_2 (solid), liquid oxide solution (designated Lox in the program), C (solid), TiC (solid or liquid), TiN (solid or liquid). The presence of each condensed phase is indicated by a flag, to be set as described under Flags.

Based on the values of the master variables and the equilibrium constant of formation, the mole number of each species is computed. Then the material balance in the elements O, N, C, and Ti is written in terms of these mole numbers. When liquid oxide is present, the stoichiometric condition is that the sum of the activities (that is, mole-fractions) of the components of the solution should add to unity; this condition replaces the atom balance in titanium for this case. There thus results a set of up to four simultaneous nonlinear equations; this set is the basis of the Newton-Raphson scheme to find the unknown parameters.

At the conclusion of an iteration, the newly generated values of the master variables are used to repeat the calculations. In favorable situations, each iteration results in improvement (although temporary divergence sometimes occurs). Iteration is repeated until the stoichiometric errors are less than one part in ten thousand.

Newt solves the set of simultaneous nonlinear equations needed to find the master variables. The Newton-Raphson method is used. In this subroutine it is necessary to find a number of derivatives numerically by observing the effect of a fractional change in each variable. This fractional change is set initially at 0.1. It is found that divergences which would otherwise occur when the errors are large can be averted by altering this fractional change to 0.5. This is accomplished by the use of special function key k8, when the computer is in a pause mode or is waiting for input. Depressing k8 a second time will change the fraction back to 0.1. The fractional errors in the stoichiometric conditions may be observed by the use of k1 (TRACE VARIABLES Yn(*)/EXECUTE) after which will be displayed Y(1),

Y(2), etc., which are these fractional errors. The display of these will remain on the screen if PRT ALL is locked down.

Approx: To begin the calculation an initial approximation of the master variables is needed. In this approximation an arbitrary hierarchy of oxygen and nitrogen uptake is assumed. Oxygen is assumed to be taken up in the order CO, titanium oxides, H_2O , CO_2 . If there is insufficient oxygen to form TiO , then TiN is assumed to be present. With excess C, C (solid) or TiC are assumed.

It has been found that **Approx** gives quite satisfactory values of the master variables at temperatures below about 3000 K; at higher temperatures the initial approximation may be in considerable error. After each entry into **Temp** the question is asked, "Do you want 'Approx'?" The default condition (obtained by pressing CONT) is "Y" for a new concentration (C/M or C + M) and "N" otherwise.

Flags sets the flags for condensed phases and gives the values of the temporary variables used in **Newt**. The criteria for the presence of a condensed phase are that the quantity of the phase, if previously computed, be nonnegative and that the formation constant be satisfied or exceeded. In the case of liquid oxide, the formation-constant requirement is replaced by the requirement that the temperature be above the melting-point curve ($T = 2143$ is used for simplicity; see text for discussion of this point) and that the sum of the activities of the components of the solution be no less than unity.

Two important indexes are set by **Flags**. **liflag** gives the number of metal-plus-oxide phases (no greater than two); for liquid oxide solution, **liflag** = 1 except that, when TiC , C (solid), and liquid oxide are all present, **liflag** = 0. The index **li** gives the number of unknowns to be sought in **Newt**. Finally **Flags** gives initial values of the variables to be used in **Newt**.

Fx gives the fitting functions for **Newt**. There are three branches, depending on the value of **liflag**. Certain of the master variables are computed in **Fx**. After **Diff** is called, the current mole numbers of all species are generated. The subroutine returns to **Newt** the variable **Fx**, which is the fractional error in the stoichiometry in whichever element **Newt** is considering at the time.

Diff first computes those master variables which were not found in **Fx**. Then **Spec** and **Oxides** are called to compute the mole numbers of all species, and finally the errors in stoichiometry for all elements (and the sum of activities when liquid oxide is present) are computed.

Spec computes the mole numbers of all gaseous species, given the current values of X, Z, Acc, and Ti. $Y = \sqrt{H_2}$ is computed in closed form in **Spec**; it is needed for computations on hydrogen-containing species. For each species the appropriate formation equilibrium constant is used.

Oxides computes the mole numbers of condensed metal and oxide phases. For two such phases (**liflag** = 2) the atom balance conditions for titanium and oxygen are used; for **liflag** = 1, only the titanium balance is used; for **liflag** = 0 the oxygen balance is used.

Nw1 serves to route the computation to the proper portions of Tical. On first entry, the flags will have been set and control is sent to Newt; except, if $li = 0$, provision exists for a closed-form solution. In either case, Flags is called again. If any flag has changed, the computation must be repeated for the new set of condensed phases; otherwise preparation is made for exit from Tical at the line Energy.

Energy computes from the stored parameters the molar internal energy of each component and then the total change in internal energy (dU) from the starting materials, taking into account the mole numbers of each species present. If the system is at the melting point of any of the condensed phases present, the amounts of solid and liquid are computed from the energy balance, using the known energy of fusion. Control is then returned to the main program.

DIAGNOSTICS

Sum1 is called at the end of each run to report the following items: (1) a check on the material balance of each element; (2) the activity of carbon (Acc) and the sum of the activities of the components of the liquid oxide solution; (3) a comparison of the computed amounts with the equilibrium constants of formation for each condensed phase; and (4) the activities (mole-fractions) of each component in the liquid oxide solution.

Sum is called whenever special function key k0 has been depressed once. At each emergence from Newt the mole numbers of all species are presented in condensed form; this is followed by Sum1, the output of which has been just described. These checks are of particular interest in troubleshooting. Depressing k0 a second time will cancel calling up Sum.

Depressing k1 will cause execution of TRACE VARIABLES $Yn(*)$. Then during each iteration in Newt the relative error functions used to test convergence will be displayed. Each $Yn(*)$ must drop below 0.0001 for convergence. This feature may be turned off by executing NORMAL.

Appendix B PROGRAM LISTING FOR "TIF4"

```

10 FILE NAME "TIF4" 22 Feb 84 | T1 + air + fuel; continuous liquid phase
20 | Adiabatic overpressure calculation (constant volume)
30
40 OPTION BASE 1
50 OVERLAP
60 ASSIGN #3 TO "THT1"
70 READ #3,1
80 DIM Xn(5),Yn(5),Xt(5),Dt(5),B(5,5),In(5,5),Mold(50),Mn(2),Xp(50)
90 DIM N(50),Ah(50,6),K(50),Du(50,5),Fob(50),Tb(1),P(50),Name(50),U(50)
100 INTEGER Cflag,Tinflag,Ticflag
110 INTEGER C(50),I,J,K,L,Mw,Cu,Mwct,In,Flag0,Flag1,Flag2,Flag3,Flag4
120 INTEGER J1,Iof,Iofuel,Check,F00,F10,F20,F30,F40,C0,Tin0,Tic0
130 DIM C=CON | Index for gases
140 G(5)=C(13)=C(14)=C(28)=0
150 FOR I=19 TO 23
160 G(I)=0
170 NEXT I
180 FOR I=35 TO 50
190 G(I)=0
200 NEXT I
210 READ #3,Ah(5),Du(5),Fob(5)
220 LOAD KEY "INDEX"
230 DISP "FOR ALL N(I) PRESS K0; FOR TRACE VARIABLES Yn(5): K1"
240
250 PAUSE
260 DEF FNGD(A,B,C)=(-B+SQRT(B^2-4*AC))/2/A
270 DEF FNS1=T1*(T1+T12+T1p) | Sum gaseous T1 atoms
280 DEF FNS=T1+C0+Qh+H2o+No+O+Hco+Hcu+Ch2o+2*(Co2+O2+T1e2) | Sum gaseous O atoms
290 DEF FNUa=Moa-FNS0 | Sum condensed O
300 DEF FNTsum=T1+2*OT12+2*OT13+T14 | Sum T1 oxides
310
320 C_m=0
330 Cpm=1 | Default total mass is 4.1 kg/cu m.
340 U=1 | Default final volume is 1.0 cu m.
350 P0=U | Default mode is constant volume
360 Cpm=M=1 | Initial nominal values
370 Eps=1E-4 | Fractional error for convergence
380 Dlt=.1 | Fractional change in variable to compute derivative
390 | Dlt may be changed to or from .5 by key KB
400
410
420 Fuel: INPUT "Name of compound",M0
430 DISP "Formula, as atoms per mole of C, H, N, O in order";
440 DISP "use k7 for TNT";
450 INPUT Ac,Ah,An,Ao
460 Mw=M(21)=M(22)=Tic=M(19)=M(20)=Tin=M(43)=M(44)=Cr=M(23)=Cu=0
470 Cu=Mw=Flag0=Flag1=Flag2=Flag3=Flag4=Cflag=Tinflag=Ticflag=0
480 | Flags and condensed phases reset for new fuel
490 IF Ac=0 THEN Ac=1E-10
500 IF Ah=0 THEN Ah=1E-10 | Provide for fuel with no C or no H
510 DISP "Internal energy of formation, J/mole";
520 DISP "use SHIFT k7 (=123) for TNT";
530 INPUT Um
540 Fms=Ac812.0115+Ah81.808+An814.8867+Ao815.9991 | Formula mass, g/mole
550
560 Conc: OUTPUT 16;"Nominal C+H = ",Cpm
570 IF Fms=0 THEN Fms=1E-10
580 INPUT "Total concentration, kg/cu m of air, C+H",Cpm
590 OUTPUT 16;"Nominal C/H = ",C_m
600 INPUT "Ratio of fuel to metal, C/H",C_m
610 PRINTER IS 7,1
620 PRINT "Total conc = ",Cpm
630 M1=Cpm/(1+C_m) | Total mass of titanium
640 Mf=Cpm-M1 | Mass of fuel
650 Cu=Mw=0 | Counter for iterations and criterion for "Approx"
660 Anp=ROUND(An,-3)
670 Acp=ROUND(Ac,-3)
680 Ahp=ROUND(Ah,-3)
690 App=ROUND(Ao,-3)
700 Up: P0=U
710 U=1
720 Conc: PRINT USING Inc:M1,Mf,Mw,Acp,Ahp,App,App,C_m
730 Inc:PAGE //,207.3D" kg of T1",2K,207.3D" kg of ",K1,C1,K1" H",K1" M",K1" O",K2X"C/M= ",3DZ.3D/
740 M1=M1/7.8679 | Moles of T1
750

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NWC TP 6544

```

760 Exit: Moles=MAX(100000/FMS,1E-10)
770 FMS=ROUND(FMS,-3)
780 Mo=ROUND(Moles,5)
790 Mi=ROUND(Mi,5)
800 PRINT Mi: " moles of Ti"
810 PRINT "Formula mass of fuel is":FMS:"g/mole. present are":Mi:"moles"
820 PRINT "VOLUME = "V:" cu m"
830 Conco: N(6)=4836: Argon
840 Nc=AcHols
850 Nn=AnHols
860 Nn=AnHols+62.96: Includes moles of N atoms from air
870 Nn=AnHols+16.951:
880 Lf=1: Default value. TIC and graphite not both present.
890 U=0: Resets internal energy
900 Ti=U=0: for temperature interpolation
910 Ais="N": Default: manual temperature setting
920 IF Ais(1)="" THEN Temp
930 T=400: for automatic temperature setting
940 GOTO Temp1
950
960 Temp: IF Flag0 THEN DISP "T=1933":
970 IF Flag1 THEN DISP "T=2023":
980 IF Flag2 THEN DISP "T=2112":
990 IF Flag3 THEN DISP "T=2047":
1000 IF Flag4 THEN DISP "T=2143":
1010 IF TicFlag THEN DISP "T=3290":
1020 IF TinFlag THEN DISP "T=3220":
1030
1040 INPUT "Approximate temperature":T
1050 INPUT "Do you want 'Approx'?(Y/N)":T
1060
1070
1080 IF UPC(ITS)="" THEN Nn=0
1090 IF UPC(ITS)="" THEN Nn=1
1100 Tn=""
1110
1120 Temp1:
1130 Calc: COSUB Eo: Computes equilibrium constants at T
1140 DISP "T": Subroutine calculates mole numbers and residual Delta U.
1150 COSUB Tical:
1160 Dn="T high":
1170 IF Dn(1) THEN Dn="T low":
1180 DISP Dn
1190
1200 FIXED 6
1210 PRINT "T =":T:" K", "Delta U =":Dn:" J", LIN(2)
1220 DISP "T =":T:" K", "Delta U =":Dn:" J"
1230 DISP Dn
1240 STANDARD
1250 IF Dn=0 THEN Ex
1260 T2=T1
1270 U2=U1
1280 Ti=T1
1290 U1=Dn
1300 IF T2(1) THEN Temp2
1310 IF Ais(1)="" THEN Temp2
1320 T=3500-500*SGN(Dn)
1330 GOTO Temp1
1340 Temp2: IF ABS(Dn)<1000 THEN Ex
1350 IF Ais="" THEN Intol
1360 DISP "To exit, press K2: Manual temperature: K4":
1370 DISP "Interpolation: CONT":
1380 PAUSE
1390 Intp: T=T2-U2*(T2-T1)/(U2-U1): Linear interpolation
1400 GOTO Calc
1410
1420 Ex: Nnum=Nn=0
1430 FOR I=1 TO 44
1440 N=Ni+N(I): Total moles of products
1450 Nnum=Nnum+C(I)*N(I): Moles of gas
1460 NEXT I
1470 ConC3:Nq=Nnum: Moles of gas
1480 Mass=(N1+Mf+1.1692)*1000: Total mass in grams
1490 Mass=Mass-59.918746-47.98181-63.98111-147.08712
1500 Mass=Mass-223.79713-79.98714-61.91811-12.81186r
1510

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```

1520 M.G=MWg/Mg I      Avg molar mass of gases
1530 N=MWg/MH I      Avg molar mass of all products
1540 PRINT USING Incon1T
1550 Incon1: IMAGE /"T = ",4D.0,"K"
1560 FIXED 3
1570 PRINT "Avg Molar mass(gases) = ";M.G;" g/mol";
1580 PRINT SPA(2);"Avg Molar mass(react) = ";N;" g/mol";
1590 PRINT SPA(5);Mg1" moles of GAS ";M1;" moles TOTAL";LIN(1)
1600 P=8.3143E-5*Mo*RT/V      RT/V, VALUE IN BARS
1610 PRINT LIN(1);"Overpressure = ";P-1;" bars";LIN(2)
1620 STANDARD
1630 PRINT "Species",SPA(8);"Moles",SPA(9);"Mole %",SPA(4);"Part. pres.";
1640 PRINT SPA(4);"LGT(K)";SPA(6);"LGT(P)";LIN(1)
1650 Final output
1660 FOR I=1 TO 34
1670 IF C(I)=0 THEN Conc5
1680 IF N(I)=0 THEN M(I)=1E-90
1690 PRINT USING Incon3;F0(I),M(I),1000N(I)/Mg,M(I)*P/Mg,LGT(N(I)/Mg),LGT(N(I)*P/Mg)
1700 Incon3: IMAGE 8A,5X,2.3DE,5X,2D.4D,5X,3D.4D,5X,ND2.3D,5X,ND2.3D
1710 Conc5: NEXT I
1720 Incon1: IMAGE 8A,5X,2.3DE,5X,2.3DE,"moles"
1730 FOR I=19 TO 23
1740 IF M(I)=0 THEN Conc6
1750 PRINT USING Incon1;F0(I),M(I)
1760 Conc6: NEXT I
1770 FOR I=35 TO 44
1780 IF M(I)=0 THEN Conc7
1790 PRINT USING Incon1;F0(I),M(I)
1800 Conc7: NEXT I
1810 Comp1: GOSUB Sum1
1820 PRINT USING Incon1;M1,Mf,Mb,Ap,Ap,Ap,Ap,C_m
1830 PRINT USING Incon1;P-1,V
1840 Incon1: IMAGE "T = ",4D.0," Overpressure = ",3D.3D," bars", " Volume = ",3D.3D," cu m"
1850 PRINT LIN(4)
1860 BEEP
1870 INPUT "DO YOU WISH TO RUN ANOTHER CONCENTRATION (Y/N)?" C9
1880 PRINT PAGE
1890 IF C9="Y" THEN Conc
1900 INPUT "Another fuel? (Y/N)" C90
1910 IF UPC0(C90)="Y" THEN Fval
1920 OUTPUT 10;"END OF ROUTINE"
1930 STOP
1940 I *****
1950 Eq) ***** COMPUTES Kn FROM LGT(Kp) PARAMETERS *****
1960 *****
1970 V=121888V/T I V/RT FOR CONST VOL = V CU M.
1980 FOR I=1 TO 50
1990 Lqk=AK(I,1)+AK(I,2)/(T+AK(I,3))+AK(I,4)*T
2000 Lqk=Lqk+AK(I,6)*LGT(V/V1)
2010 IF (I/36) AND (I/41) THEN Lqk=Lqk/2
2020 Conversion from Kp to Kn
2030 IF I=43 THEN Lqk=M1N(Lqk,99)
2040 K(1)=10*Lqk
2050 NEXT I
2060 K1c=K(19)
2070 IF T(3290) THEN K1c=K(20)
2080 K1=K(21)
2090 IF T(1933) THEN K1=K(22)
2100 K1=K(35)
2110 IF T(2023) THEN K1=K(36)
2120 K2=K(37)
2130 IF T(2112) THEN K2=K(38)
2140 K3=K(39)
2150 IF T(2047) THEN K3=K(40)
2160 K4=K(41)
2170 IF T(2143) THEN K4=K(42)
2180 K1n=K(43)
2190 IF T(3220) THEN K1n=K(44)
2200 K043=(K3/K4)*4/K1/K4
2210 K032=K2/K10*(K2/K30K20*(K2/K3))^3
2220 K031=K10*(K1/K11)*8*(K1/K11)*8*(K1/K3)*K1/K3
2230 These last 3 used for Lox calcul.
2240 RETURN I

```

```

2250 ! *****
2260 Tical) PRINT LIN(2) ! *****
2270 ! WILL FIND ALL MOLE NUMBERS AND THEN COMPUTE ENERGY BALANCE.
2280 ! *****
2290 Cu=0 ! Counts iterations
2300 IF Nw THEN Nw1
2310 Ncc=Nc
2320 Nn=Nn
2330 ! *****
2340 Approx: ! (Based mostly on condensed phases) *****
2350 ! *****
2360 FOR I=1 TO 48
2370 N(I)=0
2380 NEXT I
2390 Ar=N(6)=.4036
2400 Flag0=Flag1=Flag2=Flag3=Flag4=Tinflag=Yicflag=Lexflag=0
2410 Z=SQR(Nn/2) ! Applies when Tinflag=0
2420 IF Nn=Nc THEN Apex
2430 Co=Nn ! No oxides
2440 Yicflag=1
2450 IF Nt1>Ncc-Nn THEN Appn
2460 Cflag=1 ! Graphite present, no metal.
2470 Acc=1
2480 X=Co/Acc/K(7)
2490 Ti=N(1)=1/Acc/Xtic
2500 GOTO Appx
2510 !
2520 Appn:Flag0=1 ! Metal present, no graphite
2530 Ti=1/Kt1
2540 Acc=1/Ti/Ntic
2550 X=Co/X/K(7)
2560 GOTO Appx
2570 !
2580 Apex:Co=Ncc ! Metal oxides present
2590 IF Nt1(Nn-Ncc) THEN App1
2600 Flag1=1 ! Excess Ti: Ti-Ti0
2610 Tinflag=1
2620 Ext1=Nt1-Nn-Ncc-Nn ! The excess of Ti(c) over N
2630 IF Ext1>0 THEN App2
2640 IF Ktin/K1K2/K1K2/K1>1 THEN App3a
2650 Z=SQR(-Ext1/2) ! N is in excess: TiN + TiO
2660 Ti=N(1)=1/Ktin/Z
2670 !
2680 App3:X=1/K1/Ti
2690 GOTO Appx
2700 !
2710 App2:Flag0=1 ! Y(c) is in excess over N
2720 Ti=Ktin(Ext1.1/Kt1)
2730 Z=1/Ktin/Ti
2740 GOTO App3
2750 !
2760 App1:IF Nt1<2*(Nn-Ncc)/3 THEN App4
2770 X=K1K1/K2/K2 ! TiO Ti2O3 region
2780 Flag1=Flag2=1
2790 Ti=1/K1/X
2800 IF Ktin/K1K2/K1K2/K1<1 THEN Appx
2810 Tinflag=1
2820 Z=1/Ktin/Ti ! TiN + 2 oxides
2830 IF Nt1-2*(Nn-Ncc)/3>Nn THEN Appx
2840 IF 6*LOG(K3)+LOG(Ktin)>10*LOG(K2) THEN App4a
2850 !
2860 App4a:Z=SQR((Nn-Nt1+2*(Nn-Ncc)/3)/2) ! TiN + Ti2O3
2870 Ti=1/Ktin/Z
2880 X=(1/K2/Ti)^(2/3)
2890 GOTO Appx
2900 !

```

```

2910 App4: IF Nt1<.68*(Naa-Ncc) THEN App5
2920   X=(K2/K3)*48K28K2
2930   Flag2=Flag3=1
2940   T1=1/K2/K/SQR(X)
2950   IF 68LOG(K3)+LOG(K+1n)<18LOG(K2) THEN App4
2960   T1nflag=1
2970   Z=1/K1n/T1
2980   IF Nt1-38*(Naa-Ncc)/5>Nn THEN App4
2990   !
3000 App4a: Z=SDR((Nn-Nt1+38*(Naa-Ncc)/5)/2)
3010   T1=1/K1n/Z
3020   X=(1/K3/T1/SQR(T1))*.4
3030   GOTO App4
3040   !
3050 App5: IF Nt1<((Naa-Ncc)/2) THEN App6
3060   Flag3=Flag4=1
3070   X=K3/K4/K4/K48K3
3080   !
3090 App7: T1=1/K4/X/X
3100   !
3110 App4: Acc=Co/X/K(7)
3120   A13=T1*38X*54K38K3
3130   GOSUB Oxides
3140   GOSUB Flags
3150   GOTO Nw1
3160   !
3170 App6: Flag4=1
3180   IF Naa>Nc+28Nt1+Nn/2 THEN App6
3190   H2a=Naa-(Nc+28Nt1)
3200   H2=Nh/2-H2a
3210   X=H2a/H2/K(12)
3220   GOTO App7
3230   !
3240 Appc: IF Naa>28(Nc+Nt1)+Nn/2 THEN Appc
3250   Co2=Naa-Nc-28Nt1-Nn/2
3260   Co=Ncc-Co2
3270   X=(7)8Co2/Co/K(8)
3280   GOTO App7
3290   !
3300 Appd: Co2=Nc
3310   O2=Naa/2-(Ncc+Nt1)-Nn/4
3320   X=SQR(O2)
3330   Co=(7)8Co2/X/K(8)
3340   GOTO App7
3350 ! *****
3360 ! *      Set-up for Newton's method calculation      *
3370 ! *****
3380 Nw1:
3390   Nn=Nu+1
3400   IF I1 THEN Nw3
3410   PRINT "Closed-form calculation!"
3420   GOSUB F12
3430   GOSUB P1f1g
3440   GOSUB Dspflg
3450   IF Check THEN GOSUB Sum
3460   GOTO Nw2
3470 Nw3: GOSUB Nw1
3480 Nw2: GOSUB Flags
3490   IF (T1nflag<>T1n0) OR (Flag8<>F00) OR (Flag1<>F10) THEN Nw1
3500   IF (Flag2<>F20) OR (Flag3<>F30) OR (Flag4<>F40) THEN Nw1
3510   IF (T1cflag<>T1c0) OR (CFlag<>C0) THEN Nw1
3520   IF (Lexflag=Lex0) AND (Lflag=L0) THEN Energ
3530   !
3540   GOTO Nw1

```

T1203 - T1305 region
 T1N + 2 oxides
 T1N + T1305
 T1305 - T102 region
 Exit from "Approx"
 (Initial approx.)
 T102 + H2O
 HC - H2O mixture
 CO - CO2 mixture
 Excess O2
 Controls entry into "Approx"
 "Nw1" not used in this case
 If any flag changes, iterations are repeated.

```

3550 | #####
3560 | * PRINT FLAG STATUS *
3570 | #####
3580 Prtflg: IF Tinflag THEN PRINT " TIN";
3590 IF Ticflag THEN PRINT " TIC";
3600 IF Cflag AND (Ac)IE-10 THEN PRINT " Gr";
3610 IF Laxflag OR Lflag THEN PRINT " Lex"; " (" ; LF; ")";
3620 IF Flag0 THEN PRINT " Net";
3630 IF Flag1 THEN PRINT " T10";
3640 IF Flag2 THEN PRINT " T1203";
3650 IF Flag3 THEN PRINT " T1305";
3660 IF Flag4 THEN PRINT " T102";
3670 PRINT TAB(1)
3680 RETURN
3690 | #####
3700 | DISPLAY FLAG STATUS
3710 | #####
3720 Dispflg: DISP TAB(1) Display flag status
3730 DISP "NEWTON'S CALC. ", SPA(5);
3740 IF Tinflag THEN DISP " TIN";
3750 IF Ticflag THEN DISP " TIC";
3760 IF Cflag AND (Ac)IE-10 THEN DISP " Gr";
3770 IF Laxflag OR Lflag THEN DISP " Lex"; " (" ; LF; ")";
3780 IF Flag0 THEN DISP " Net";
3790 IF Flag1 THEN DISP " T10";
3800 IF Flag2 THEN DISP " T1203";
3810 IF Flag3 THEN DISP " T1305";
3820 IF Flag4 THEN DISP " T102";
3830 RETURN
3840 | #####
3850 Newt: A NEWTON'S METHOD FOR UP TO FIVE SIMULTANEOUS NON-LINEAR EQNS
3860 | #####
3870 READIN Xn(I), Yn(I), Xt(I), Delx(I), D(I), I1, In(I), I1)
3880 GOSUB Dispflg
3890 Newt0: Cu=0 Counter for Newton's method iterations
3900 Newt0: Cu=0 Counts entries into Newt
3910 Newt3: MAT X=Xn
3920 PRINTER IS 7,1
3930 Cu=Cu+1
3940 FOR I=1 TO I1
3950 K=J
3960 GOSUB Fx
3970 Yn(I)=Fx
3980 FOR J=1 TO I1
3990 K=J
4000 Xt(J)=(1-Dlt)*Xn(J)
4010 GOSUB Fx
4020 D(I,J)=-(Fx-Yn(I))/Xn(J)/Dlt
4030 Xt(J)=Xn(J)
4040 NEXT J
4050 NEXT I
4060 IF DET(D)() THEN Newt1
4070 PRINT "MATRIX SINGULAR"
4080 DISP "MATRIX SINGULAR"
4090 PRINTER IS 0
4100 PRINT LIN(1), "D Matrix:"
4110 MAT PRINT D
4120 PRINT LIN(1)
4130 GOSUB Sum
4140 STOP
4150
4160 Newt1: MAT In=INV(D)
4170 MAT Delx=In*Yn
4180 MAT Xn=Xn-Delx
4190 Newt4: FOR I=1 TO I1
4200 IF Xn(I)=0 THEN Newt2
4210 Xn(I)=(Xn(I)+Delx(I))/2!
4220 Newt2: NEXT I
4230 Newt2: NEXT I
4240 FOR I=1 TO I1
4250 IF ABS(Yn(I))Eps THEN Newt3
4260 GOSUB Fx
4270 NEXT I
4280 PRINT Cu; " ITERATIONS FOR "; I1; " VARIABLES; ";
4290 GOSUB Prtflg
4300 PRINTER IS 7,1
4310 IF Check=0 THEN RETURN
4320 GOSUB Sum
4330 Retn: RETURN

```

If (= 0, use 1/2 previous value

Diagnostics given when Check=0 (given by key K0)

```

4340 *****
4350 Flags: ***** Sets flags, i.e. initial values for Neut *****
4360 *****
4370 ***** Sets flags for condensed phases.
4380 ***** Formation constants must be exceeded
4390 ***** and amount of phase not negative
4400
4410 Tin0=Tinflag ! To save old values
4420 Lox=Lflag
4430 Lox0=Loxflag
4440 F00=Flag0
4450 F10=Flag1
4460 F20=Flag2
4470 F30=Flag3
4480 F40=Flag4
4490 Tic0=Ticflag
4500 C0=Cflag
4510 Cflag=MIN(1,INT(Acc))*(Gr)=0
4520 IF Gr=0 THEN Gr=0
4530 IF Acc=1E-10 THEN Cflag=1 ! For fuels with no carbon
4540 Ticflag=(TicAcc*(Tic)-1E-5)*(Tic)=0*(Acc)=1E-10
4550 IF Tic=0 THEN Tic=0
4560 Lf=NOT (Ticflag AND Cflag) ! Lf=1 unless Tic and graphite both present
4570 Tinflag=(Tin0*(Tin)-1E-5)*(Tin)=0
4580 IF Tin=0 THEN Tin=0
4590 Flag0=(Tic0*(Tic)-1E-5)*(Tic)=0
4600 IF Tin=0 THEN Tin=0
4610 Flag1=(Tic0*(Tic)-1E-5)*(Tic)=0
4620 IF Tin=0 THEN Tin=0
4630 Flag2=(Tic0*(Tic)-1E-5)*(Tic)=0
4640 IF Tin=0 THEN Tin=0
4650 Flag3=(Tic0*(Tic)-1E-5)*(Tic)=0
4660 IF Tin=0 THEN Tin=0
4670 Flag4=(Tic0*(Tic)-1E-5)*(Tic)=0
4680 IF Tin=0 THEN Tin=0
4690 COSUB Act
4700 Loxflag=(Tic0*(Tic)-1E-5)*(Tic)=0
4710
4720
4730 IF Lox=0 THEN Lox=0
4740 IF Loxflag THEN Flag0=Flag1=Flag2=Flag3=Flag4=0
4750 Lflag=Loxflag AND Lf
4760 IF Lflag THEN Loxflag=0 !
4770
4780 Tcon=NTI-FMSi-Tin !
4790 Ocon=Non-FMSi !
4800 IF NOT (Cflag AND Flag1) THEN Flag0
4810 Cflag=(Ncc)/MIN(Tcon,Ocon)/3 !
4820 Flag1=1-Cflag
4830 Flag2=Ticflag=1
4840 Flag3=1-Flag1
4850 Flag4=1-Flag2
4860 Flag5=(Tcon)/3*(Ncc)
4870 Ticflag=1-Flag3
4880 Flag6=1-Flag4
4890 Flag7=1-Flag5
4900 Ticflag=(2*Ocon)/3*(Tcon)
4910 Flag4=1-Ticflag
4920 Flag1:IF (Ticflag=1) OR (Flag0=0) OR (Cflag=0) OR (Acc=1E-10) THEN I1set
4930 Flag0=(NTI-FMSi)/Ncc ! With TIC, either Met or Gr, not both
4940 Cflag=1-Flag0
4950
4960 I1set:I1flag=Flag0+Flag1+Flag2+Flag3+Flag4+Lflag ! I1flag can be 0, 1, or 2.
4970 ! I1flag = 1 for Lflag but 0 for Loxflag
4980 IF I1flag=2 THEN Flag1
4990 I1=4-I1flag-Tinflag-Ticflag-Cflag ! Number of variables in "Neut"
5000 IF I1=0 THEN RETURN
5010 REDIM Xn(I1)
5020 ! Following sets values of variables in "Neut"
5030 IF NOT Tinflag THEN Xn(I1)=2
5040 IF NOT Tinflag AND NOT Cflag AND NOT Ticflag THEN Xn(I1)=Acc
5050 IF Tinflag AND NOT Cflag AND NOT Ticflag THEN Xn(I1)=Acc
5060 IF I1flag=2 THEN Xn(I1)=X
5070 IF (I1flag=1) AND Tinflag AND NOT Flag0 AND NOT Loxflag AND NOT Lflag THEN Xn(I1)=Ti
5080 IF (I1flag=0) AND NOT (Cflag AND Ticflag) THEN Xn(I1)=Ti
5090 RETURN
5100 !
5110 ! The variables are X (if no more than one oxide or metal),
5120 ! Ti (if no oxide or metal) and 2 (if TiN is absent).
5130 ! Exception: When TiN and one solid oxide, but no metal or liquid oxide
    present then Ti (and not X) is first variable.

```

```

5140 Flag1=Tcon=Nti-FNSti-Tin-Tic
5150 IF Iiflag=4 THEN F14
5160 IF NOT Flag0 AND NOT Flag1 THEN F13a
5170 IF NOT Flag0 AND NOT Flag4 THEN F13b
5180 IF NOT Flag3 AND NOT Flag4 THEN F13c
5190 IF Qcon)Tcon THEN F14
5200 Flag0=Flag1
5210 Flag2=Flag3=Flag4=0
5220 GOTO I1set
5230 F1a: Flag0=0
5240 GOTO F14a
5250 F14: IF NOT Flag0 THEN F14a
5260 IF NOT Flag0 THEN F14a
5270 F13c: Flag2=(Qcon)Tcon
5280 Flag0=NOT Flag2
5290 GOTO I1set
5300 F13b: Flag0=Flag4=0
5310 Flag3=(Qcon)1.6*Tcon
5320 Flag1=NOT Flag3
5330 GOTO I1set
5340 F14a: IF Qcon=1.5*Tcon THEN F13b
5350 Flag1=0
5360 F13a: Flag4=(Qcon)5*Tcon/3
5370 Flag2=NOT Flag4
5380 GOTO I1set
5390 Fx: ***** Fitting functions for Newton's method calc. *****
5400 *****
5410 *****
5420 *****
5430 *****
5440 *****
5450 *****
5460 *****
5470 *****
5480 *****
5490 *****
5500 *****
5510 *****
5520 IF NOT Tinflag THEN Z=Xt(I1)
5530 IF NOT Tinflag AND NOT Cflag AND NOT Ticflag THEN Acc=Xt(I1-1)
5540 IF Tinflag AND NOT Cflag AND NOT Ticflag THEN Acc=Xt(I1)
5550 ON Iiflag+1 GOTO Fx0,F11,Fx2
5560
5570 Fout:GOSUB Diff
5580
5590 IF (I=1) AND (Iiflag=2) THEN Fx=D0/N0a
5600 IF (I=1) AND (Iiflag=1) AND Tinflag AND NOT Lflag AND NOT Flag0 THEN Fx=Dti/Nti
5610 IF Loxflag AND ((I=2) OR (I=1) AND Cflag AND Ticflag) THEN Fx=Atsum-1
5620 IF (I=2) AND NOT Iiflag AND NOT Lflag THEN Fx=Dti/Nti
5630 IF NOT Tinflag AND (I=1) THEN Fx=Dein/Nn
5640 IF NOT Tinflag AND NOT Cflag AND NOT Ticflag AND (I=1-1) THEN Fx=Deic/Nc
5650 IF Tinflag AND NOT Cflag AND NOT Ticflag AND (I=1) THEN Fx=Deic/Nc
5660
5670 RETURN
5680
5690 Fx0: X=Xt(I1)
5700 IF NOT (Cflag AND Ticflag) THEN Ti=N(I1)=Xt(2)
5710 IF Cflag AND Ticflag THEN Ti=N(I1)=1/Ktic
5720 IF NOT Loxflag THEN Fout
5730 GOSUB Act
5740 GOTO Fout
5750 *****
5760 Act: ***** Give activities in liquid oxide *****
5770 *****
5780 At=Kt1Xt1
5790
5800 At1=K1T1X
5810 At2=T1&T1XXXXXXK2&K2
5820 At3=T1&T1&T1&XXXXXXK3&K3(Lflag=2)
5830 At4=K4T1X
5840 Atsum=At0+At1+At2+At3+At4
5850 RETURN
5860 *****

```

The case of Iiflag=2, which is disallowed

The case of Iiflag=5

For Iiflag =4

Flags 0,1,2

Flags 1,2,3

Iiflag = 4, Flag0 = 0

Flags 2,3,4

"Fx" computes errors in stoichiometric conditions for existing values of variables.
Finds appropriate values of master variables
Calls on "Soec" to compute moles of all species
Xt(i) is used, since both original value of variable and value changed by Dit are employed.

Exit routine for "Fx"
Following are stoichiometric conditions to use in "Newt"

The stoichiometric tests correspond with the variables.
Returns to "Newt" (or to "Nu" for Ii=0)

For Iiflag=0

Activity of metal in liquid oxide
Following are activities of oxides in liquid oxide

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```

5870 Fx1:
5880 IF Tinflag AND NOT Flag0 AND NOT Lflag THEN Fx1a
5890 X=Xt(1)
5900 IF NOT Lflag THEN Fx1b
5910 !
5920 !
5930 A3=-1/K3/K3/X/X/X/X/X
5940 A2=-(K1+K1X+K4XX)A3
5950 A1=-XXXXK2K2A3 !
5960 Ar=(3A2-A1A1)/3
5970 Br=(2A1A1A1-9A1A2)/27+A3 !
5980 Dc=BrBr/4+ArArAr/27 !
5990 IF Dc=0 THEN Fx1c
6000 R1=-Br/2+SQR(Dc)
6010 R1=SGN(R1)*SGN(R1)*R1^(1/3) !
6020 R2=-Br/2-SQR(Dc)
6030 R2=SGN(R2)*SGN(R2)*R2^(1/3)
6040 Xr=R1+R2 !
6050 Ti=N(1)*Xr-A1/3
6060 IF Ti=0 THEN Fout
6070 Fx1c: IF Lflag THEN Ti=N(1)=FNOD(X0X0K2K2,K1+K1X+K4XX,-1)
6080 !
6090 Lf=2
6100 GOTO Fout
6110 Fx1b: !
6120 IF Flag0 THEN Ti=N(1)=1/Kt1
6130 IF Flag1 THEN Ti=N(1)=1/K1/X
6140 IF Flag2 THEN Ti=N(1)=1/K2/X/SQR(X)
6150 IF Flag3 THEN Ti=N(1)=(1/K3/X/X/SQR(X))^(2/3)
6160 IF Flag4 THEN Ti=N(1)=1/K4/X/X
6170 IF NOT (Cflag AND Ticflag) THEN Fout
6180 Z=Xt(1) !
6190 Ti=N(1)=1/Ktic
6200 X=(1/K2/Ti)^(2/3)
6210 GOTO Fout
6220 Fx1a: Ti=N(1)=Xt(1) !
6230 IF Flag1 THEN X=1/K1/Ti
6240 IF Flag2 THEN X=(1/K2/Ti)^(2/3)
6250 IF Flag3 THEN Y=(1/K3/Ti/SQR(Ti))^4
6260 IF Flag4 THEN X=SQR(1/K4/Ti)
6270 GOTO Fout
6280 !
6290 Fx2: IF NOT (Flag0 AND Flag1) THEN Fx2a
6300 Ti=N(1)=1/Kt1 !
6310 X=1/Ti/K1
6320 GOTO Fout
6330 Fx2a: IF NOT (Flag1 AND Flag2) THEN Fx2b
6340 X=K1/K2K1/K2 !
6350 Ti=N(1)=1/K1/X
6360 GOTO Fout
6370 Fx2b: IF NOT (Flag2 AND Flag3) THEN Fx2c
6380 X=(K2/K3)^4K2K2 !
6390 Ti=N(1)=1/K2/X/SQR(X)
6400 GOTO Fout
6410 Fx2c: IF NOT (Flag3 AND Flag4) THEN Fx2d
6420 X=K3/K4/K4/K4K3
6430 Ti=N(1)=1/K4/X/X
6440 GOTO Fout
6450 Fx2d: IF NOT (Flag2 AND Flag4) THEN Fx2e
6460 X=K2/K4K2/K4
6470 Ti=N(1)=1/K4/X/X
6480 GOTO Fout
6490 Fx2e: IF Cflag AND Flag1 AND NOT Ticflag THEN Alert2
6500 Ti=1/Ktic
6510 X=1/K1/Ti
6520 GOTO Fout !

```

For Lflag =1

For Lflag=1, solves a cubic to find $Ti = f(X)$
Must satisfy sum of activities = 1

Coeff. of cubic (Unit coeff. for cubic term.)

Reduced cubic, lacks quadratic.
Discriminant of the cubic

Avoids cube roots of negative no.

The only real root of the reduced eqn.

In case cubic had negative root

Case of TiC + graphite + $Ti2O3$

For TiH + $Fe2$ oxide

$Ti - TiO$ region

$TiO - Ti2O3$ region

$Ti2O3 - Ti2O5$ region

```

6530 ! *****
6540 ! Diff; Calculates error functions for C, O, N, H2 and H2O *****
6550 ! *****
6560 ! Diff:
6570 IF Tinflag THEN Z=1/Ti/Ktin
6580 IF Ticflag THEN Acc=1/Ti/Ktic
6590 GOSUB Spec
6600 Tin=(Nnc-No-2NH2)*Tinflag
6610 Tic=(Ncc-Co-Co2)*Ticflag
6620 !
6630 N(44)=Tin*(T(3220)
6640 N(43)=Tin-N(44)
6650 N(20)=Tic*(T(3290)
6660 N(19)=Tic-N(20)
6670 GOSUB Oxides ! GIVES OXIDES AND METALS
6680 Dri=Nti-FNSti-Tin-Tic-Met-FNisum
6690 D2=Non-FNSe-Ti1-3*Ti2-5*Ti3-2*Ti4
6700 Deln=Nnc-No-2NH2-Tin
6710 IF Cflag AND Ticflag THEN Tic=Dri+Tic
6720 Delc=Ncc-Co-Co2-Tic
6730 Cr=N(23)=Delc/Cflag*(Ac)1E-10)
6740 RETURN
6750 !
6760 ! *****
6770 ! ***** Computes moles of all gaseous species *****
6780 ! *****
6790 ! Spec: Input: X, Ti, Z, Acc
6800 O2=N(18)=X^2
6810 O=N(17)=K(17)*X
6820 TiO=N(2)=K(2)*Ti*X
6830 TiO2=N(3)=K(3)*Ti*X*X
6840 !
6850 N2=N(16)=2*Z
6860 N=N(15)=K(15)*X*X
6870 MgO=N(42)=K(42)*Mg*X
6880 !
6890 ! Car: IF Cflag THEN Acc=1
6900 IF Acc=1E-10 THEN Acc=1E-30 ! For fuels with no carbon
6910 Co=N(7)=K(7)*Acc*X
6920 CO2=N(8)=K(8)*Acc*X*X
6930 H2=N(9)=K(9)*X+Acc*(K(29)*Z+K(30)*Z*X+K(31)*X*X+2*Acc*Acc)
6940 !
6950 ! Coefficient of monohydrogen species
6960 ! Coefficient of dihydrogen species
6970 H=N(19)=K(9)*X
6980 H2=N(11)=X*X
6990 H2O=N(12)=K(12)*X*X*X
7000 Hcn=N(29)=K(29)*Acc*X*X
7010 Hnci=N(30)=K(30)*Acc*X*X*X
7020 Hco=N(31)=K(31)*Acc*X*X
7030 Ch2o=N(32)=K(32)*Acc*X*X*X
7040 C2h2=N(33)=K(33)*Acc*Acc*X*X
7050 TiO=N(4)=Cnn=N(24)=50R(K(4)*K(24)*Ti*Acc*Z)
7060 Cn=N(25)=K(25)*Acc*Z
7070 C2n=N(26)=K(26)*Acc*Acc*Z
7080 C2n=N(27)=K(27)*Acc*Acc*Z
7090 C3=N(34)=K(34)*Acc*Acc*Acc
7100 Ncc=Nc-Hcn-Hnci-Hco-Ch2o-Cn-Cnn-2*(C2h2+C2h+C2n)-3*C3
7110 !
7120 Nnc=Mn-Hcn-Hnci-(N-C2n-Cnn)
7130 IF Nnc(0) THEN Nnc=1E-50
7140 RETURN !

```


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```

7150 ! *****
7160 ! ***** Moles of metals and oxides *****
7170 ! *****
7180 Oxides: FOR In=19 TO 22
7190     N(In)=0
7200     NEXT In
7210     FOR In=35 TO 44
7220         N(In)=0
7230     NEXT In
7240     Met=T11=T12=T13=T14=0
7250     !
7260     IF NOT Iiflag AND NOT Loxflag THEN RETURN
7270     Tcon=Nti-FNSfi-Tin-Tic !
7280     Ocon=Nou-FNSo !
7290     IF Loxflag OR Lflag THEN Oxlx
7300     IF Iiflag=1 THEN Oxi
7310     !
7320     IF NOT (Flag0 AND Flag1) THEN Oxb
7330     T11=Ocon
7340     Met=Tcon-T11
7350     GOTO Ox2
7360     !
7370 Oxb: IF NOT (Flag1 AND Flag2) THEN Oxc
7380     T12=Ocon-Tcon
7390     T11=Tcon-2*T12
7400     GOTO Ox2
7410     !
7420 Oxc: IF NOT (Flag2 AND Flag3) THEN Oxd
7430     T13=2*Ocon-3*Tcon
7440     T12=(Tcon-3*T13)/2
7450     GOTO Ox2
7460     !
7470 Oxd: IF NOT (Flag3 AND Flag4) THEN Oxe
7480     T13=2*Tcon-Ocon
7490     T14=Tcon-3*T13
7500     GOTO Ox2
7510     !
7520 Oxe: IF NOT Flag2 AND Flag4 THEN Alert2
7530     T12=2*Tcon-Ocon
7540     T14=Tcon-2*T12
7550     GOTO Ox2
7560 Oxi: IF Tinflag THEN Oxtin
7570     IF Flag0 THEN Met=Tcon !
7580     IF Flag1 THEN T11=Tcon
7590     IF Flag2 THEN T12=Tcon/2
7600     IF Flag3 THEN T13=Tcon/3
7610     IF Flag4 THEN T14=Tcon
7620     GOTO Ox2
7630     !
7640 Oxtin: IF Flag0 THEN Met=Tcon-Nnc+No*2*N2 !
7650     IF Flag1 THEN T11=Ocon
7660     IF Flag2 THEN T12=Ocon/3
7670     IF Flag3 THEN T13=Ocon/5
7680     IF Flag4 THEN T14=Ocon/2
7690     GOTO Ox2
7700     !
7710 Oxlx: Sumox=Tcon/((1+A1+2*A2+A3))
7720     IF Cflag AND Ticflag THEN Sumox=Ocon/((1+2*A1+4*A2+A3+A4))
7730     !
7740     GOSUB Act
7750     Met=At0*Sumox
7760     T11=At1*Sumox
7770     T12=At2*Sumox
7780     T13=At3*Sumox
7790     T14=At4*Sumox
7800     Lox=Met+T11+T12+T13+T14 !
7810     !
7820 Ox2: N(22)=Met*(T(1933))
7830     N(21)=Met-N(22)
7840     N(36)=T11*(T(2023))
7850     N(35)=T11-N(36)
7860     N(38)=T12*(T(2112))
7870     N(37)=T12-N(38)
7880     N(40)=T13*(T(2647))
7890     N(39)=T13-N(40)
7900     N(42)=T14*(T(2143))
7910     N(41)=T14-N(42)
7920     RETURN !

```

Preceding prevents carryover of old values

Condensed Ti + oxides
Condensed O

Following for two oxides or metal + one oxide

For Iiflag = 1, no liquid oxide

Routine for Tin + one oxide. This line is not bal in N.

Liquid oxide present

For this case use 0 rather than Ti balance

Moles of liquid oxide

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```

7930 : #####
7940 : ##### Energy: Computes Delta U #####
7950 : #####
7960 Energy: Du=-U
7970 FOR I=1 TO 44
7980   U(I)=Du(I,1)+Du(I,2)*T+Du(I,3)*T*T+Du(I,5)/T+Du(I,4)*LOG(T)
7990   !
8000   Du=Du+U(I)*N(I)!
8010   NEXT I
8020   IF Du=0 THEN RETURN
8030   IF Flag0 AND (T=1933) THEN En0
8040   IF Ticflag AND (T=3290) THEN Entic
8050   IF Flag1 AND (T=2023) THEN En1
8060   IF Flag2 AND (T=2112) THEN En2
8070   IF Flag3 AND (T=2147) THEN En3
8080   IF Flag4 AND (T=2143) THEN En4
8090   IF Tinflag AND (T=3220) THEN Entin
8100   RETURN !
8110   !
8120   !
8130   Entic: N(20)=Du/71145 !
8140   N(19)=MAX(0,Tic-N(20)) !
8150   Du=Du*(N(19)=0)
8160   IF N(19) THEN RETURN
8170   N(20)=Tic
8180   GOTO Enbeep
8190   En0: N(22)=Du/18623 !
8200   N(21)=MAX(0,Net-N(22)) !
8210   Du=Du*(N(21)=0)
8220   IF N(21) THEN RETURN
8230   N(22)=Net
8240   GOTO Enbeep
8250   Entin: N(44)=Du/66960 !
8260   N(43)=MAX(0,Tin-N(44)) !
8270   Du=Du*(N(43)=0)
8280   IF N(43) THEN RETURN
8290   N(44)=Tin
8300   GOTO Enbeep
8310   En1: N(36)=Du/54405 !
8320   N(35)=MAX(0,Ti1-N(36)) !
8330   Du=Du*(N(35)=0)
8340   IF N(35) THEN RETURN
8350   N(36)=Ti1
8360   GOTO Enbeep
8370   En2: N(38)=Du/110484 !
8380   N(37)=MAX(0,Ti2-N(38)) !
8390   Du=Du*(N(37)=0)
8400   IF N(37) THEN RETURN
8410   N(38)=Ti2
8420   GOTO Enbeep
8430   En3: N(40)=Du/138105 !
8440   N(39)=MAX(0,Ti3-N(40)) !Liquid Ti305
8450   Du=Du*(N(39)=0)
8460   IF N(39) THEN RETURN
8470   N(40)=Ti3
8480   GOTO Enbeep
8490   En4: N(42)=Du/65960 !
8500   N(41)=MAX(0,Ti4-N(42)) !
8510   Du=Du*(N(41)=0)
8520   IF N(41) THEN RETURN
8530   N(42)=Ti4
8540   !
8550   Enbeep: BEEP
8560   DISP "Select a lower temperature"
8570   RETURN !

```

```

8580 ! *****
8590 ! ***** Diagnostics *****
8600 ! *****
8610 Alert2: ! Improper oxides present
8620 PRINT "Error in OXIDES"
8630 GOSUB Sum
8640 STOP
8650 GOTO Temp
8660 !
8670 !
8680 Sum: ! PRINTER IS 7,1 ! If activated by K1, prints after each iteration
8690 GOSUB Spec
8700 GOSUB Ptf1g
8710 PRINT LIN(1), "T = ", T, LIN(1)
8720 I=1
8730 PRINT USING Insum; F0(I), N(I), F0(I+1), N(I+1), F0(I+2), N(I+2), F0(I+3), N(I+3)
8740 I=4
8750 PRINT USING Insum; F0(I), N(I), F0(I+1), N(I+1), F0(I+2), N(I+2), F0(I+3), N(I+3)
8760 I=10
8770 PRINT USING Insum; F0(I), N(I), F0(I+1), N(I+1), F0(I+2), N(I+2), F0(I+3), N(I+3)
8780 I=15
8790 PRINT USING Insum; F0(I), N(I), F0(I+1), N(I+1), F0(I+2), N(I+2), F0(I+3), N(I+3)
8800 I=24
8810 PRINT USING Insum; F0(I), N(I), F0(I+1), N(I+1), F0(I+2), N(I+2), F0(I+3), N(I+3)
8820 I=28
8830 PRINT USING Insum; F0(I), N(I), F0(I+1), N(I+1), F0(I+2), N(I+2), F0(I+3), N(I+3)
8840 I=33
8850 PRINT USING Insum; F0(I), N(I), F0(I+1), N(I+1)
8860 PRINT USING Insum; "TiC", Tic, "Met", Met, "TiO", Ti1, "T.233", Ti2
8870 PRINT USING Insum; "Ti3O5", Ti3, "TiO2", Ti4, "TiN", Tin, "Gr", Gr
8880 Insum: ! IMAGE J(84, KZ, DDE, 3X)
8890 Sum: ! Sum=FNSi+Tin+Tic+Met+FNTsum ! Added up in final output
8900 PRINT LIN(1), "Ti BALANCE ", Wt1, Sum
8910 Sum=FNSi+Ti1+3*Ti2+5*Ti3+2*Ti4
8920 PRINT "O BALANCE ", Wt0, Sum
8930 Sum=Tin+2*H2+No+Hcn+Hnce+Cn+C2n+Cnn
8940 PRINT "N BALANCE ", Wn, Sum
8950 Sum=Nc+Ncc+Ca+Co2+Tic+Gr
8960 PRINT "C balance ", Wc, Sum
8970 Sum=Hn+H+2*H2+H2O
8980 PRINT "H balance ", Wn, Sum
8990 PRINT USING "K,K"; "Acc= ", Acc
9000 PRINT USING "K,K, /"; "Atsum = ", Atsum
9010 PRINT LIN(2); TAB(20); "Test for equilibrium", LIN(1)
9020 PRINT SPA(1), "K"; TAB(10); "Numeric"; TAB(30);
9030 PRINT "Functional(=Numeric)". LIN(1)
9040 FLOAT Z
9050 IF NOT Loxflag AND NOT Lflaq THEN A*0=At1=At2=At3=A*4=1
9060 PRINT "Ti0"; TAB(10); At0/Kt1; TAB(30); Ti
9070 PRINT "Ti0"; TAB(10); At1/K1; TAB(30); TiX
9080 PRINT "Ti2O3"; TAB(10); SQR(At2)/K2; TAB(30); TiXXSQR(Y)
9090 PRINT "Ti3O5"; TAB(10); SQR(At3)/K3; TAB(30); TiXXXSQR(TiXX)
9100 PRINT "TiO2"; TAB(10); At4/K4; TAB(30); TiXO2
9110 PRINT "TiN"; TAB(10); 1/Ktin; TAB(30); TiX2
9120 PRINT "TiC"; TAB(10); 1/Ktic; TAB(30); TiXAcc
9130 IF Loxflag OR Lflaq THEN PRINT LIN(1)
9140 IF Loxflag OR Lflaq THEN PRINT USING Insum; "a(Met)", A*0, "a(TiO)", At1, "a(Ti2O3)", At2
9150 IF Loxflag OR Lflaq THEN PRINT USING Insum; "a(Ti3O5)", At3, "a(TiO2)", At4
9160 ! Activities in liquid oxide
9170 STANDARD
9180 PRINTER IS 7,1
9190 RETURN

```

NWC TP 6544

```

9200 | #####
9210 | ##### Species, codes, and flags #####
9220 | #####
9230 | #####
9240 | #####
9250 | 1 Ti
9260 | 2 TiO
9270 | 3 TiO2
9280 | 4 Ti+
9290 | 5 (not used)
9300 | 6 Au
9310 | 7 CO
9320 | 8 CO2
9330 | 9 H
9340 | 10 OH
9350 | 11 H2
9360 | 12 H2O
9370 | 13 (not used)
9380 | 14 (not used)
9390 | 15 NO
9400 | 16 N2
9410 | 17 O
9420 | 18 O2
9430 | 19 TiO(l)
9440 | 20 TiO(s)
9450 | 21 Ti(l)
9460 | 22 Ti(s)
9470 | 23 C(s)
9480 | 24 CN-
9490 | 25 CN
9500 | 26 C2H
9510 | 27 C2N
9520 | 28 (not used)
9530 | 29 HCN
9540 | 30 HNCN
9550 | 31 HCO
9560 | 32 CH2O
9570 | 33 C2H2
9580 | 34 C3
9590 | 35 TiO(l)
9600 | 36 TiO(s)
9610 | 37 Ti2O3(l)
9620 | 38 Ti2O3(s)
9630 | 39 Ti3O5(l)
9640 | 40 Ti3O5(s)
9650 | 41 TiO2(l)
9660 | 42 TiO2(s)
9670 | 43 TiN(l)
9680 | 44 TiN(s)
9690 |
9700 |
9710 | Loxflag or Lflag indicates presence of continuous liquid phase
9720 | At0, At1, At2, At3, At4 for activity (ideal solution)
9730 | of Met, TiO, Ti2O3, Ti3O5, TiO2
9740 | Acc = activity of carbon
9750 | X = SQR(O2)
9760 | Y = SQR(H2)
9770 | Z = SQR(N2)
9780 |
9790 | Variables used in Newton's method calculation:
9800 | No metal or oxide X,Ti
9810 | One oxide only/metal only X (Ti if TiN + i solid oxide, no metal)
9820 | Two oxides/metal + i oxide -
9830 | In all cases, Z and Acc are the last two variables when appropriate
9840 | END

```

CODE	FLAG	FORMATION CONST
19	TiO(l)	Tic
20	TiO(s)	Ticflag
21	Ti(l)	Met
22	Ti(s)	Met
23	C(s)	Gr
35	TiO(l)	Ti1
36	TiO(s)	Ti1
37	Ti2O3(l)	Ti2
38	Ti2O3(s)	Ti2
39	Ti3O5(l)	Ti3
40	Ti3O5(s)	Ti3
41	TiO2(l)	Ti4
42	TiO2(s)	Ti4
43	TiN(l)	Tin
44	TiN(s)	Tin

NWCTP 6544

KEY 0
Check=(Check+1)
-Execute

KEY 1
TRACE VARIABLES Yn(8)
-Execute

KEY 2
CONT Ex
-Execute

KEY19
-Clear line
SCRATCH

KEY 4
CONT Temp
-Execute

KEY 5
Attn="y"
-Execute

KEY 6
TRACE PAUSE 5
-Execute

KEY 7
2,5,3,6
-Continue

KEY 8
 $D1t=.48(D1t+.1)+.1$
-Execute

KEY 9
-Clear line
LOAD

KEY10
-Clear line
SAVE

KEY11
-Clear line
STORE

KEY12
-Clear line
EDIT

KEY13
-Clear line
EDIT LINE

KEY14
-Clear line
LIST

KEY15
-Clear line
SCRATCH

KEY23
-11750
-Continue

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